Finite Volume Effects in Chiral Perturbation Theory with Twisted Boundary Conditions

Inauguraldissertation
der Philosophisch-naturwissenschaftlichen Fakultät
der Universität Bern

vorgelegt von

Alessio Giovanni Willy Vaghi

von Chiasso

Leiter der Arbeit: Prof. Dr. G. Colangelo
Albert Einstein Center
for Fundamental Physics
Institut für theoretische Physik
Universität Bern

Original document saved on the web server of the University Library of Bern

This work is licensed under a
Creative Commons Attribution-Non-Commercial-No derivative works 2.5 Switzerland licence.
To see the licence go to http://creativecommons.org/licenses/by-nc-nd/2.5/ch/ or write to
Creative Commons, 171 Second Street, Suite 300, San Francisco, California 94105, USA.

Finite Volume Effects in Chiral Perturbation Theory with Twisted Boundary Conditions

Inauguraldissertation
der Philosophisch-naturwissenschaftlichen Fakultät
der Universität Bern

vorgelegt von

Alessio Giovanni Willy Vaghi

von Chiasso

Leiter der Arbeit: Prof. Dr. G. Colangelo
Albert Einstein Center
for Fundamental Physics
Institut für theoretische Physik
Universität Bern

Von der Philosophisch-naturwissenschaftlichen Fakultät angenommen.

Der Dekan:

Bern, den 17. Dezember 2015

Prof. Dr. G. Colangelo

Copyright Notice

This document is licensed under the
Creative Commons Attribution-Non-Commercial-No derivative works 2.5 Switzerland.
http://creativecommons.org/licenses/by-nc-nd/2.5/ch/

You are free:

to copy, distribute, display, and perform the work

Under the following conditions:

Attribution. You must give the original author credit.

Non-Commercial. You may not use this work for commercial purposes.

No derivative works. You may not alter, transform, or build upon this work.

For any reuse or distribution, you must take clear to others the license terms of this work.

Any of these conditions can be waived if you get permission from the copyright holder.

Nothing in this license impairs or restricts the author's moral rights according to Swiss law.

The detailed license agreement can be found at:
http://creativecommons.org/licenses/by-nc-nd/2.5/ch/legalcode.de

To my grandmother and my parents.

The Force is what gives a Jedi his power. It's an energy field created by all living things. It surrounds us and penetrate us. It binds the galaxy together.

Alec Guinness as Ben "Obi-Wan" Kenobi,
in *Star Wars Episode IV: A New Hope*

Abstract

We study the effects of a finite cubic volume with twisted boundary conditions on pseudoscalar mesons. We apply Chiral Perturbation Theory in the p-regime and introduce the twist by means of a constant vector field. The corrections of masses, decay constants, pseudoscalar coupling constants and form factors are calculated at next-to-leading order. We detail the derivations and compare with results available in the literature. In some case there is disagreement due to a different treatment of new extra terms generated from the breaking of the cubic invariance. We advocate to treat such terms as renormalization terms of the twisting angles and reabsorb them in the on-shell conditions. We confirm that the corrections of masses, decay constants, pseudoscalar coupling constants are related by means of chiral Ward identities. Furthermore, we show that the matrix elements of the scalar (resp. vector) form factor satisfies the Feynman–Hellman Theorem (resp. the Ward–Takahashi identity). To show the Ward–Takahashi identity we construct an effective field theory for charged pions which is invariant under electromagnetic gauge transformations and which reproduces the results obtained with Chiral Perturbation Theory at a vanishing momentum transfer. This generalizes considerations previously published for periodic boundary conditions to twisted boundary conditions.

Another method to estimate the corrections in finite volume are asymptotic formulae. Asymptotic formulae were introduced by Lüscher and relate the corrections of a given physical quantity to an integral of a specific amplitude, evaluated in infinite volume. Here, we revise the original derivation of Lüscher and generalize it to finite volume with twisted boundary conditions. In some cases, the derivation involves complications due to extra terms generated from the breaking of the cubic invariance. We isolate such terms and treat them as renormalization terms just as done before. In that way, we derive asymptotic formulae for masses, decay constants, pseudoscalar coupling constants and scalar form factors. At the same time, we derive also asymptotic formulae for renormalization terms. We apply all these formulae in combination with Chiral Perturbation Theory and estimate the corrections beyond next-to-leading order. We show that asymptotic formulae for masses, decay constants, pseudoscalar coupling constants are related by means of chiral Ward identities. A similar relation connects in an independent way asymptotic formulae for renormalization terms. We check these relations for charged pions through a direct calculation. To conclude, a numerical analysis quantifies the importance of finite volume corrections at next-to-leading order and beyond. We perform a generic analysis and illustrate two possible applications to real simulations.

Contents

Introduction

General Overview

As far as we know, there are four fundamental interactions in nature: gravitational, weak, electromagnetic and strong interactions. Their ranges of action and their strengths are remarkably different, as one can see from Tab. 1. The gravitational interaction (or gravitation) is essential for the existence of galaxies, planetary systems, stars (and for our everyday life) but at subatomic distances is so feeble that can be neglected. The weak interaction plays a fundamental role in many subatomic processes as e.g. the β-decay of the neutron. The electromagnetic interaction (or electromagnetism) appears in all phenomena involving electric charges or radiation of the frequency comprised between radio waves and gamma rays. The strong interaction holds together protons and neutrons within the nucleii of atoms and is the strongest interaction at the distance of 1 fm.

The strong interaction is also responsible for the formation of hadrons. Hadrons are bound states formed by quarks and gluons (fundamental particles of unknown substructure) and are classified in two groups: baryons and mesons. In the simplest description, baryons are triplets of quarks bound together via gluon exchanges whereas mesons are quark-antiquark pairs. The best known baryons are the proton p and the neutron n which are commonly referred to as nucleons, $\mathcal{N} = \{ p, n \}$. Mesons are less familiar: the best known are pions, kaons and eta which are all members of the subgroup of pseudoscalar mesons. In this work, we study the lightest pseudoscalar mesons and the effects on their physical properties of a finite volume. Apart from being an interesting subject on its own, the

Table 1: The four fundamental interactions, their ranges of action and their relative strengths at the distance of one femtometre, i.e. $1\ \mathrm{fm} = 10^{-15}\ \mathrm{m}$. *Note that gravitational and electromagnetic interactions have an infinite range of action and may act at all distances.*

Interaction	Range [fm]	Relative strength
Gravitational	∞	10^{-38}
Weak	100	10^{-6}
Electromagnetic	∞	10^{-2}
Strong	1	1

study of finite volume effects is mainly motivated by a specific research area of Theoretical Particle Physics, namely Lattice QCD. This area has greatly progressed in the last few years and in the future, will allow one to solve Quantum Chromodynamics completely from first principles.

Over the years, Quantum Chromodynamics (or QCD) has been established as the fundamental theory describing the strong interaction. It was formulated during 1970es as a relativistic quantum field theory relying on Quantum Mechanics and Special Relativity. Since then, it has been precisely tested, becoming a part of the successful Standard Model of Particle Physics. However, QCD still poses some theoretical challenges. At high energies, the theory is worked out with the standard approach used in quantum field theories: perturbation theory. The coupling constant serves as an expansion parameter and physical observables are expanded in its powers. As long as the coupling constant is small, the expansion converges and the results of physical observables can be compared with experimental measurements. This provides precise tests on the validity of the theory. At low energies, the coupling constant is however not small. The terms of the expansion, instead of becoming smaller, get bigger and bigger leading to divergent expressions. In that case, standard perturbation theory fails and alternative methods must be applied in order to solve the theory.

Already in Ref. [1] Wilson proposed an alternative approach, known as Lattice QCD. He discretized the space-time and formulated QCD on a 4-dimensional lattice. The lattice acts twofold. On one hand, it serves as a regulator, rendering the theory finite. On the other hand, it enables calculations of physical observables through numerical simulations. Lattice QCD is so simulated on computers and solved with the help of Monte Carlo techniques. It turns out that such task is challenging even for the powerful computers of the last generation. Firstly, because Monte Carlo techniques rely on sophisticated algorithms that often, do not succeed to simulate the light quarks at their physical masses. Secondly, because the computational power needed to solve the theory grows rapidly as the lattice approaches a continuum space-time of infinite extent. In practice, most of the simulations are performed with light-quark masses larger than in nature ($\hat{m} > \hat{m}^{\text{phys}}$) on cubic lattices with a coarse site spacing ($a > 0$) and a finite extent ($L < \infty$). To give a rough estimate, present-day simulations feature: $\hat{m} \approx 10$—20 MeV, $a \approx 0.05$—0.1 fm and $L \approx 2$—4 fm, see Ref. [2]. Hence, to compare the results of such simulations with real experiments one has to take three extrapolations: $\hat{m} \to \hat{m}^{\text{phys}}$, $a \to 0$ and $L \to \infty$. These extrapolations are by no means straightforward and must be guided in some way.

Another method to treat QCD at low energies are effective field theories. This method is rather old: first simplest applications are due to Fermi, Euler and Heisenberg around mid-1930s, see Ref. [3–7]. The rigorous mathematical formulation came solely 40 years later with the decoupling Theorem of Appelquist–Carazzone [8] and the Weinberg Theorem [9]. Towards mid-1980s Gasser and Leutwyler applied the method to QCD and relying on a few general principles, they constructed an effective field theory for pions [10] which was extended to other pseudoscalar mesons in Ref. [11]. This effective theory is mainly based on an approximate symmetry of QCD (the so-called chiral symmetry) and is named after that as Chiral Perturbation Theory.

Chiral Perturbation Theory (ChPT) is the low-energy effective field theory of QCD. It approximates QCD at low energies where "low" means under the scale $\Lambda_\chi \approx 1$ GeV. Below this scale, ChPT is mathematically equivalent to QCD and allows one to perform perturbative calculations. Physical observables are expanded in powers of small external momenta and light-quark masses according to an expansion which is known as chiral expansion. The chiral expansion is formally different from the expansion of standard perturbation theory. In particular, it involves low-energy constants that are not determined by the effective theory itself and must be determined in other ways. Already in Ref. [10, 11] Gasser and Leutwyler determined about twenty of them, comparing theoretical results with the phenomenology of the strong interaction. Since then, many calculations have been done in ChPT and many extensions for its theoretical framework have been proposed, see e.g. Ref. [12–18]. The picture that emerges 30 years later, is a substantial success of this effective field theory.

Nowadays, Lattice QCD and ChPT are mature research areas of Theoretical Particle Physics. It is not uncommon that they are combined together to provide a joined analysis. Specifically, Lattice QCD can pin down the low-energy constants of the chiral expansion and in turn, ChPT can guide the extrapolations of numerical simulations. In this respect, the present work deals with the infinite volume extrapolation ($L \to \infty$). Herein, we study finite volume effects and determine the L-dependence of various physical observables applying ChPT in finite volume. Knowing the algebraic form of the L-dependence is essential to extrapolate the results of numerical simulations. In Ref. [19–21] Gasser and Leutwyler first showed how to apply ChPT in finite volume. They proved that if the volume is large enough, the theory enters the so-called p-regime and only a few modifications must be taken into account, see Ref. [21]. Physical observables are calculated in a similar way as in infinite volume and their results are shifted by additional finite volume corrections. These corrections are L-dependent and decay exponentially as the volume gets large. In the limit $L \to \infty$, finite volume corrections disappear and the results of physical observables return as in infinite volume.

The physical origin of finite volume corrections lies in the vacuum polarization. Each real particle is surrounded by a cloud of virtual ones that polarizes the vacuum. In general, virtual particles can propagate up to distances of the extent of their Compton wavelength. If the system is enclosed in a finite volume, the cloud of virtual particles is squeezed and there is a probability that during their propagation, virtual particles encounter the boundaries and wind around the volume, before they are reabsorbed by the real particle. This winding generates the finite volume corrections and makes physical observables dependent on L.

In Ref. [22] Lüscher introduced another method to estimate finite volume corrections. He derived an asymptotic formula relating mass corrections to an integral of a specific scattering amplitude, evaluated in infinite volume. A detailed derivation was then presented in Ref. [23] where Lüscher succeeded to generalize the proof to all orders in perturbation theory by means of Abstract Graph Theory. Successively, the formula was widely applied in combination with ChPT [24–30] and extended to other quantities such as decay constants [31, 32] and pseudoscalar coupling constants [31]. In these applications, ChPT provided oneself with the analytic representation for the amplitudes entering the integrands of asymptotic formulae. Knowning such representation at a given order, it is then possible to numerically estimate the corrections at one order higher. This is a very convenient aspect of asymptotic formulae as they automatically push the estimation of corrections to higher orders.

In this work, we study finite volume effects by means of ChPT and asymptotic formulae. We consider finite cubic volumes with twisted boundary conditions [33–36] which are a generalization of the periodic ones. Twisted boundary conditions are usually imposed in lattice simulations to introduce continuous momenta that were otherwise not allowed by the periodic ones. In this way, it is possible to extract specific physical quantities which are defined from continuous limits such as e.g. square radii or curvatures of form factors. Note that results obtained with twisted boundary conditions can be always reduced to the case with the periodic ones just by setting the twist equal to zero.

Structure of the Work

In Chapter 1 we present ChPT. We first outline the method of effective field theories: we summarize its general principles and sketch the construction of effective theories in practice. Then, we apply the effective method to QCD at low energies. We give a short introduction on QCD highlighting its symmetry properties and construct the effective chiral Lagrangian of ChPT. The chapter ends with four applications of ChPT: we calculate masses, decay constants, pseudoscalar coupling constants and form factors at NLO in the chiral expansion.

In Chapter 2 we study ChPT in finite volume. We give an overview of finite volume effects and introduce twisted boundary conditions. Then, we calculate finite volume corrections at NLO. We start with the corrections of masses and decay constants for which we detail the derivations of pions (corrections of other pseudoscalar mesons can be analogously derived). We compare the expressions with the results of Ref. [36, 37] and outline the main differences with Ref. [38]. From these expressions, we calculate the corrections of pseudoscalar coupling constants by means of chiral Ward identities [10, 11]. We check with the results obtained through the direct calculation [38] and confirm that they are in agreement. Successively, we calculate the corrections of the matrix elements of pion form factors. We compare the expressions with Ref. [37, 38] and show that in this case, the Feynman–Hellman Theorem [39, 40] and the Ward–Takahashi identity [41–43] hold in finite volume with twisted boundary conditions.

Chapter 3 begins with an overview of asymptotic formulae. We outline the method and recall the asymptotic formulae of pseudoscalar mesons valid in finite volume with periodic boundary conditions. Then, we revise the original derivation of Lüscher [23] and generalize it to twisted boundary conditions. We derive asymptotic formulae for masses, decay constants, pseudoscalar coupling constants and scalar form factors. The formulae for scalar form factors are derived relying on the Feynman–Hellman Theorem [39, 40] and are then valid at vanishing momentum. Furthermore, we show that the asymptotic formulae for masses, decay constants, pseudoscalar coupling constants are related by means of chiral

Ward identities. We check these relations for charged pions through a direct calculation combining results of ChPT with asymptotic formulae.

In Chapter 4 we apply asymptotic formulae in combination with ChPT. To express the amplitudes entering the formulae, we take the chiral representation at one loop from Ref. [10, 44–48]. We work out this representation for the kinematics needed in the asymptotic formulae and expand them beyond NLO. The results are presented in terms of integrals in a similar way as Ref. [32].

Chapter 5 summarizes the numerical analysis. We first discuss the numerical set-up and perform a generic analysis. The corrections are evaluated numerically at NLO using the expressions obtained with ChPT in Chapter 2 and then, estimated beyond NLO using the asymptotic formulae of Chapter 4. Results are presented by means of graphs representing the dependences on the pion mass and on the twisting angles. Successively, we illustrate two possible numerical applications to real simulations. We take lattice data from two collaborations [49–51] and estimate finite volume corrections at NLO and beyond NLO.

The Appendices contain further details on analytical aspects. Appendix A is a list of results that may be useful for the evaluation of loop diagrams in finite volume. In Appendix B we study the (electromagnetic) gauge symmetry in finite volume. We first construct an effective theory for charged pions which is invariant under gauge transformations and which reproduces results obtained with ChPT in Chapter 2. As the gauge symmetry is here preserved, we show that the Ward–Takahashi identity [41–43] holds in finite volume if the momentum transfer is discrete. Such considerations were previously presented in Ref. [52] and in this work, are generalized to the case with twisted boundary conditions. In Appendix C we introduce some concepts of Abstract Graph Theory and generalize the first part of the derivation of Lüscher [23] to twisted boundary conditions. At last, Appendix D contains some cumbersome expressions of the integrals presented in Chapter 4.

Chapter 1

Chiral Perturbation Theory

1.1 Effective Field Theories

Effective field theories (EFT) are a method of a wide application in Physics. There are EFT in many research areas: from Condensed Matter to Nuclear and Particle Physics as well as in General Relativity, see Ref. [53–57]. Most of them are low-energy approximations: they approximate fundamental theories at energies lower than some characteristic scale Λ. Below the characteristic scale the EFT is mathematically equivalent to the underlying fundamental theory. It provides the mathematical apparatus to expand physical quantities in powers of p/Λ (or E/Λ) where p is an external momentum and E is an energy. As long as $E \ll \Lambda$ the expansion converges and the results can be compared with experiments testing the reliability of the approximation. For higher energies the expansion breaks down and one must reformulate the EFT in order to reliably approximate the fundamental theory.

The method of EFT relies on a few general principles. These were summarized by Weinberg in a folk's Theorem which was proven under specific circumstances by Leutwyler [58] as well as D'Hoker and Weinberg [59]. The Theorem states [9]: a "[...] quantum field theory itself has no content beyond analycity, unitarity, cluster decomposition and symmetry". Analycity follows from causality, i.e. after a Lorentz transformation cause and effect cannot change their time ordering. Unitarity guarantees the probability conservation postulated by Quantum Mechanics: the theory is compatible with a description in terms of the scattering matrix S, in which an initial state i evolves in a final state f with total probability, $\sum_f |\langle f| \, S \, |i\rangle|^2 = 1$. The cluster decomposition principle ensures locality, namely that there is no mutual influence for sufficiently spatially separated experimental measurements. The word symmetry summarizes the invariance of the system under various transformations: Poincaré, charge-conjugation, parity, time reversal and internal transformations.

In practice, the construction of EFT proceeds in the following way. For a specific energy region (defined by the characteristic scale) one writes down the most general Lagrangian containing the fields of active particles and including all possible terms allowed by the symmetry of the underlying fundamental theory. Then, the perturbative expansion of the effective Lagrangian produces the most general S-matrix consistent with the principles summarized in the Weinberg Theorem [9]. In most of the cases the effective Lagrangian contains an infinite numbers of terms. However, as the Lagrangian is written for a specific energy region it is possible to order the terms according to their relevance and work (within a certain accuracy) with a finite number of them.

One can distinguish two main types of EFT relying on the transition from high energies (i.e. $E \gg \Lambda$) to low energies ($E \ll \Lambda$), see Ref. [55].

Decoupling EFT. The fundamental theory contains fields with well separated masses, $M_{l_i} \ll \Lambda \lesssim M_{H_j}$. Here, the characteristic scale corresponds to the mass of heavy fields. At low energies the degrees of freedom of heavy fields are frozen. The decoupling Theorem [8] asserts that the heavy fields H_j can be integrated out from the theory and the effective Lagrangian depends only on light fields l_i,

$$\mathcal{L}(l_i, H_j) \xrightarrow[E\ll\Lambda]{} \mathcal{L}_{\text{eff}}(l_i) = \mathcal{L}_{d\leq 4} + \sum_{d>4} \frac{1}{\Lambda^{d-4}} \sum_{k_d} g_{k_d} O_{k_d}. \tag{1.1}$$

The effective Lagrangian is split in renormalizable and non-renormalizable parts. The renormalizable part $\mathcal{L}_{d\leq 4}$ contains a finite number of terms constructed from operators of light fields. The operators have dimensionality $d \leq 4$ and are potentially renormalizable. The non-renormalizable part is an infinite series of operators O_{k_d} with an increasing dimensionality and a decreasing relevance. These operators are multiplied by negative powers of Λ and their contribution is suppressed at low energies. The coupling constants g_{k_d} are dimensionless and their values must be determined from the fundamental theory.

Non-decoupling EFT. Owing to some phase transition the degrees of freedom at low energies differ from those of the fundamental theory. An example of such phase transition is a spontaneous symmetry breaking. Here, Λ is the charateristic scale where the spontaneous symmetry breaking occurs and where new degrees of freedom –the Goldstone bosons– are generated. In the presence of a mass gap in the energy spectrum, the Goldstone bosons characterize the dynamics at low energies. The EFT is constructed in terms of their fields and according to their symmetry properties. As the spontaneous symmetry breaking relates processes involving different numbers of Goldstone bosons, the effective Lagrangian contains infinitely many terms with an arbitrary number of fields. Such Lagrangian is intrinsically non-renormalizable. However, it is still possible to order the effective Lagrangian by means of a power counting. As each derivative corresponds to a momentum of Fourier space, terms with n derivatives count as $\mathcal{O}(p^n/\Lambda^n)$. The effective Lagrangian is ordered in terms with an increasing number of derivatives and a decreasing relevance at low energies. It turns out that at a given n there are finitely many terms $\mathcal{O}(p^n/\Lambda^n)$ which can be renormalized among themselves. Thus, the effective Lagrangian is renormalizable order by order and provides finite results. An example of non-decoupling EFT is Chiral Perturbation Theory (ChPT).

Table 1.1: Flavors q_f, masses m_f and electric charges Q_e of quarks from Particle Data Group [2]. For light flavors the values of the isospin I as well as of its third component I_3 and the values of the strangeness quantum number S are additionally listed. Note that the masses of light flavors are in [MeV] *whereas those of heavy ones are in* [GeV]. *For light flavors, these values were estimated in the $\overline{\text{MS}}$ scheme with renormalization scale $\mu = 2$ GeV. For heavy flavors, the values of m_c, m_b refer to the "running" masses in the same $\overline{\text{MS}}$ scheme and the value of m_t is a combined result of measurements at Tevatron and LHC [63].*

(a) Light flavors.

q_f	m_f [MeV]	Q_e [e]	I	I_3	S
u	$2.3^{+0.7}_{-0.5}$	$+\frac{2}{3}$	$\frac{1}{2}$	$+\frac{1}{2}$	0
d	$4.8^{+0.5}_{-0.3}$	$-\frac{1}{3}$	$\frac{1}{2}$	$-\frac{1}{2}$	0
s	95 ± 5	$-\frac{1}{3}$	0	0	-1

(b) Heavy flavors.

q_f	m_f [GeV]	Q_e [e]
c	1.275 ± 0.025	$+\frac{2}{3}$
b	4.18 ± 0.03	$-\frac{1}{3}$
t	173.34 ± 0.76	$+\frac{2}{3}$

1.2 Quantum Chromodynamics

We give a short introduction to Quantum Chromodynamics [60,61]. We study its symmetry properties and discuss how the strong interaction can be described at low energies. The discussion is based on Ref. [62].

1.2.1 Gauge Invariance

Quantum Chromodynamics (QCD) is the fundamental theory underlying the strong interaction. It describes the dynamics of the strong interaction in terms of quarks and gluons, fundamental particles of the Standard Model. Quarks are spin-1/2 fermions and are represented by Dirac spinors. They occur in six flavors: up, down, strange, charm, bottom and top (in short u, d, s, c, b, t). Without going into details we list them in Tab. 1.1 and report the values of their masses as well as some quantum numbers. Gluons are spin-1 bosons and are represented by vector fields. They are massless and do not carry electric charges. In QCD there are eight gluons which may interact among themselves.

QCD describes the strong interaction among quarks and gluons by means of gauge invariance. Gauge invariance requires that the theory must be invariant under a continuous group of local transformations. In QCD the continuous group is called the color group and is represented by the set of 3×3 unitary matrices with unit determinant, $\text{SU}(3)_\text{c}$. The local transformations can be parametrized in terms of eight real continuous functions $\Theta_a(x)$ as

$$\mathcal{U}(x) = \exp\left(-i\,\Theta_a(x)\frac{\lambda_a}{2}\right) \in \text{SU}(3)_\text{c}, \qquad a = 1, \ldots, 8. \tag{1.2}$$

Here, the repetition of the index a implies a sum[1]. The matrices λ_a are the Gell-Mann matrices and act in color space,

$$\lambda_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \lambda_2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \lambda_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\lambda_4 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \quad \lambda_5 = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix} \quad \lambda_6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \tag{1.3}$$

$$\lambda_7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} \quad \lambda_8 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}.$$

According to gauge invariance the local transformations (1.2) leave the theory invariant. This implies that the QCD Lagrangian reads

$$\mathcal{L}_{\text{QCD}} = \sum_{f=1}^{N_{\text{f}}} \bar{q}_f \, (i\not{D} - m_f) \, q_f - \frac{1}{4} \, G_{\mu\nu,a} \, G_a^{\mu\nu}. \tag{1.4}$$

The index f runs over the number of flavors. In ordinary QCD there are $N_{\text{f}} = 6$ flavors and the masses m_f are free parameters. Each quark field $q_f = q_f(x)$ is a triplet in color space and transforms under the color group as

$$q_f = \begin{pmatrix} q_{f,R} \\ q_{f,B} \\ q_{f,G} \end{pmatrix} \mapsto \begin{pmatrix} q'_{f,R} \\ q'_{f,B} \\ q'_{f,G} \end{pmatrix} = \mathcal{U}(x) \, q_f. \tag{1.5}$$

The components of the triplet represent quarks of a different color charge (red, blue, green or R, B, G) but identical in all the rest. The adjoint field $\bar{q}_f := q_f^\dagger \gamma^0$ transforms under the color group as

$$\bar{q}_f \mapsto \bar{q}_f \, \mathcal{U}^\dagger(x). \tag{1.6}$$

Here, γ^0 is the Dirac gamma matrix with the Lorentz index $\mu = 0$ and acts in spinor space. The covariant derivative $\not{D} := \gamma^\mu D_\mu$ is defined so that under the color group it transforms in the same way as the quark field,

$$D^\mu q_f \mapsto \mathcal{U}(x) \, (D^\mu q_f) \, . \tag{1.7}$$

This request introduces eight gluon fields $G_a^\mu = G_a^\mu(x)$ which carry different combinations of color charges. The gluon fields generate the interaction in the Lagrangian and transform under the color group as

$$\frac{\lambda_a}{2} G_a^\mu \mapsto \mathcal{U}(x) \, \frac{\lambda_a}{2} G_a^\mu \, \mathcal{U}^\dagger(x) - \frac{i}{g} \, [\partial^\mu \mathcal{U}(x)] \, \mathcal{U}^\dagger(x), \tag{1.8}$$

[1] Unless stated otherwise, we will use this convention throughout.

where g is the strong coupling costant. In the first term of $\mathcal{L}_{\mathrm{QCD}}$, gluon fields enter through the covariant derivative

$$D^\mu = \partial^\mu - ig\,\frac{\lambda_a}{2} G_a^\mu, \tag{1.9}$$

and couple to quark fields generating the interaction among quarks and gluons. The strength of such interaction is measured by the coupling constant g. Since g is equal for all $f = 1, \ldots, N_\mathrm{f}$ gluon fields couple to quark fields independently of the flavor.

In the last term of $\mathcal{L}_{\mathrm{QCD}}$, gluon fields enter through the field-strength tensor

$$G_a^{\mu\nu} = \partial^\mu G_a^\nu - \partial^\nu G_a^\mu + g\, f_{abc}\, G_b^\mu G_c^\nu. \tag{1.10}$$

Here, f_{abc} are the structure constants of $\mathrm{SU}(3)_\mathrm{c}$. The tensor transforms under the color group as

$$\frac{\lambda_a}{2} G_a^{\mu\nu} \mapsto \mathcal{U}(x)\,\frac{\lambda_a}{2} G_a^{\mu\nu}\,\mathcal{U}^\dagger(x). \tag{1.11}$$

The term $-\frac{1}{4} G_{\mu\nu,a} G_a^{\mu\nu}$ is the simplest one that can be constructed with just gluon fields and in the respect of gauge invariance. It incorporates kinetic and self-interaction terms of gluons. The kinetic terms consist of monomials with exactly two derivatives of G_a^μ. Self-interaction terms contain either two gluon fields and a derivative of G_a^μ (describing a self interaction among three gluons) or four gluon fields (describing a four-gluon interaction). Note that there is no mass term for G_a^μ. This is excluded by construction as it would explicitly break the gauge invariance in $\mathcal{L}_{\mathrm{QCD}}$. For that reason, gluons are assumed massless.

QCD features asymptotic freedom [64–69]. This property refers to the dependence of the coupling constant on the energy (or momentum) transfer among interacting particles. In QCD the coupling constant decreases when the energy gets higher. In the asymptotic limit of extreme high energies the coupling constant is so small that quarks and gluons behave as if they were free. Still, nobody has ever directly observed a single quark or gluon [2]. Instead one observes a large variety of hadrons, i.e. bound states of quarks and gluons with no color. This is supposed to be a consequence of color confinement: the strength of the strong interaction increases with the separation distance of color charges so that two color charges can not be singularly isolated and remain confined within hadrons in configurations with no color. Color confinement has not been mathematically proven, yet. It has been proven under certain circumstances in simulations of Lattice QCD [1] but a rigourous mathematical proof still lacks [70].

Asymptotic freedom justifies the use of perturbation theory in QCD. At high energies the coupling constant is small enough and can be used as an expansion parameter. Physical observables are expanded in its powers and the results are compared with experimental measurements providing precise tests for the theory, see Ref. [2]. At low energies the situation is quite different. The coupling constant is not small enough to guarantee a perturbative expansion. One must apply alternative methods. Relying on the Weinberg Theorem [9] Gasser and Leutwyler have applied the method of EFT to low-energy QCD and have formulated Chiral Perturbation Theory [10, 11]. This effective theory allows one to perform perturbative calculations at low energies using as expansion parameters small external momenta and small masses. In the following, we will briefly introduce the basic concepts and the principal equations underlying ChPT.

1.2.2 Accidental Global Symmetry

The scale of 1 GeV is typical in the hadron spectrum. The lightest vector mesons $\{\rho,\ \omega,\ K^*, \phi\}$ the nucleons $\mathcal{N} = \{\, p, n\,\}$ and other light baryons –such as e.g. $\{\,\Lambda^0, \Sigma\,\}$– have all masses close to 1 GeV. For instance, the proton has a mass $M_p \approx 0.9383$ GeV, as reported by PDG [2]. In the simplest description, the proton is a bound state formed by three valence quarks: uud. Naively, one can sum up their masses obtaining $2m_u + m_d \approx 0.009$ GeV which is well under 1 GeV. It is clear that the masses of valence quarks contribute to M_p in a negligible way and there must be some more complicated mechanism giving the mass to the proton.

ChPT is formulated at energies lower than $\Lambda_\chi \approx 1$ GeV. From Tab. 1.1 we observe that quark masses encompass a wide range: from a few MeV up to hundreds of GeV. Taking Λ_χ as the characteristic scale, we observe that three flavors (i.e. u, d, s) are lighter than 1 GeV while the others are heavier. This is just a qualitative comparison but suffices to give the idea that at low energies (i.e. for $E \ll \Lambda_\chi$) the degrees of freedom of heavy flavors are frozen. The decoupling Theorem [8] tells us that the fields of heavy flavors can be integrated out. Hence, we just consider light flavors and set $N_\mathrm{f} = 3$ in the QCD Lagrangian. For convenience, we introduce a new notation and gather the fields of light flavors in a vector,

$$q = (q_f)_{1\le f\le 3} = \begin{pmatrix} u \\ d \\ s \end{pmatrix}, \tag{1.12}$$

while their masses in a matrix,

$$\mathcal{M} = \begin{pmatrix} m_u & 0 & 0 \\ 0 & m_d & 0 \\ 0 & 0 & m_s \end{pmatrix}. \tag{1.13}$$

With this notation the QCD Lagrangian can be rewritten as

$$\begin{aligned} \mathcal{L}_\mathrm{QCD} &= \mathcal{L}^0_\mathrm{QCD} - \bar{q}\,\mathcal{M}\,q, \\ \mathcal{L}^0_\mathrm{QCD} &= \bar{q}\,i\not{D}\,q - \frac{1}{4}\,G_{\mu\nu,a}\,G_a^{\mu\nu}. \end{aligned} \tag{1.14}$$

The Lagrangian $\mathcal{L}_\mathrm{QCD}$ describes the dynamics of the three light flavors. The kinetic terms (as well as terms of gluon fields) are contained in $\mathcal{L}^0_\mathrm{QCD}$ while the masses are accomodated in $-\bar{q}\,\mathcal{M}\,q$. The mass term $-\bar{q}\,\mathcal{M}\,q$ disappears as $m_u, m_d, m_s \to 0$. As a first approximation, we can set $-\bar{q}\,\mathcal{M}\,q$ to zero since the masses m_u, m_d, m_s are well under 1 GeV. We will reintroduce the mass term later as a small perturbation of $\mathcal{L}^0_\mathrm{QCD}$. In the following, we concentrate on $\mathcal{L}^0_\mathrm{QCD}$ and study its symmetry.

The Lagrangian $\mathcal{L}^0_{\mathrm{QCD}}$ describes the dynamics of three massless flavors. It exhibits a global symmetry in flavor space. The symmetry manifests itself in two independent subspaces defined by the chiral projections,

$$P_L = \frac{1}{2}(\mathbb{1}_4 - \gamma_5) \qquad \text{and} \qquad P_R = \frac{1}{2}(\mathbb{1}_4 + \gamma_5). \tag{1.15}$$

Here, $\mathbb{1}_4$ is the 4×4 unit matrix and $\gamma_5 = \gamma^5 = i\gamma^0\gamma^1\gamma^2\gamma^3$. The chiral projections are hermitian operators of spinor space and satisfy: the completeness relation (i.e. $P_L + P_R = \mathbb{1}_4$), the ortogonality condition ($P_L P_R = P_R P_L = 0$), the idempotence definition ($P_L^2 = P_L$ resp. $P_R^2 = P_R$). They project the quark fields in two chiral components,

$$q = P_L q + P_R q = q_L + q_R. \tag{1.16}$$

The massless Lagrangian can be rewritten as

$$\mathcal{L}^0_{\mathrm{QCD}} = \bar{q}_L\, i\not{D}\, q_L + \bar{q}_R\, i\not{D}\, q_R - \frac{1}{4}\, G_{\mu\nu,a}\, G^{\mu\nu}_a. \tag{1.17}$$

We observe that chiral components can be transformed independently from each others, leaving $\mathcal{L}^0_{\mathrm{QCD}}$ invariant. This corresponds to an invariance under the symmetry,

$$\mathrm{U}(3)_L \times \mathrm{U}(3)_R = \mathrm{SU}(3)_L \times \mathrm{SU}(3)_R \times \mathrm{U}(1)_L \times \mathrm{U}(1)_R, \tag{1.18}$$

namely under the transformations,

$$\begin{aligned} &q_L \mapsto \mathcal{V}_L\, q_L && q_R \mapsto \mathcal{V}_R\, q_R \\ &\mathcal{V}_L = \exp\left(-i\,\Theta^L_a \frac{\lambda_a}{2}\right) \mathrm{e}^{-i\,\Theta^L} \in \mathrm{U}(3)_L && \mathcal{V}_R = \exp\left(-i\,\Theta^R_a \frac{\lambda_a}{2}\right) \mathrm{e}^{-i\,\Theta^R} \in \mathrm{U}(3)_R. \end{aligned} \tag{1.19}$$

Here, λ_a are Gell-Mann matrices in flavor space and $\Theta^L, \Theta^R, \Theta^L_a, \Theta^R_a$ are 18 real constant parameters with $a = 1, \ldots, 8$.

By virtue of the Noether Theorem [71] the symmetry (1.18) implies the existence of 18 currents,

$$\begin{aligned} L^\mu_a &= \bar{q}_L \gamma^\mu \frac{\lambda_a}{2}\, q_L & R^\mu_a &= \bar{q}_R \gamma^\mu \frac{\lambda_a}{2}\, q_R \\ L^\mu &= \bar{q}_L \gamma^\mu q_L & R^\mu &= \bar{q}_R \gamma^\mu q_R, \end{aligned} \tag{1.20}$$

which are conserved at classical level,

$$\partial_\mu L^\mu_a = \partial_\mu L^\mu = \partial_\mu R^\mu_a = \partial_\mu R^\mu = 0. \tag{1.21}$$

In this case, their charges,

$$\begin{aligned} Q^L_a &= \int \mathrm{d}^3x\, L^0_a & Q^R_a &= \int \mathrm{d}^3x\, R^0_a \\ Q^L &= \int \mathrm{d}^3x\, L^0 & Q^R &= \int \mathrm{d}^3x\, R^0, \end{aligned} \tag{1.22}$$

are time independent operators and correspond to the generators of the symmetry (1.18). For convenience, we rewrite the currents as linear combinations with a definite parity

$$\begin{aligned} V_a^\mu &= L_a^\mu + R_a^\mu = \bar{q}\gamma^\mu \frac{\lambda_a}{2} q & \qquad A_a^\mu &= R_a^\mu - L_a^\mu = \bar{q}\gamma^\mu\gamma_5 \frac{\lambda_a}{2} q \\ V^\mu &= L^\mu + R^\mu = \bar{q}\gamma^\mu q & \qquad A^\mu &= R^\mu - L^\mu = \bar{q}\gamma^\mu\gamma_5 q. \end{aligned} \tag{1.23}$$

The linear combinations V_a^μ, V^μ (resp. A_a^μ, A^μ) have positive (negative) parity and transform like vector (axialvector) currents. The charges can be rewritten in an analogous way,

$$\begin{aligned} Q_a^V &= Q_a^L + Q_a^R = \int \mathrm{d}^3x\ q^\dagger \frac{\lambda_a}{2} q & \qquad Q_a^A &= Q_a^R - Q_a^L = \int \mathrm{d}^3x\, q^\dagger \gamma_5 \frac{\lambda_a}{2} q \\ Q^V &= Q^L + Q^R = \int \mathrm{d}^3x\ q^\dagger q & \qquad Q^A &= Q^R - Q^L = \int \mathrm{d}^3x\, q^\dagger \gamma_5 q, \end{aligned} \tag{1.24}$$

and have the same parity as the currents they originate from.

It turns out that at quantum level, the theory is affected by an anomaly, see Ref. [72–75]. The singlet axialvector current $A^\mu = \bar{q}\gamma^\mu\gamma_5 q$ is not conserved and its divergence values

$$\partial_\mu A^\mu = \frac{3g^2}{2(4\pi)^2}\, \epsilon_{\mu\nu\rho\sigma} G_a^{\mu\nu} G_a^{\rho\sigma}. \tag{1.25}$$

Here, $\epsilon_{\mu\nu\rho\sigma}$ is the totally antisymmetric Levi-Civita tensor and the factor 3 corresponds to the number of light flavors. The anomaly breaks the part of the symmetry corresponding to the singlet axialvector current, $\mathrm{U}(1)_A = \mathrm{U}(1)_{R-L}$. Then, the massless Lagrangian $\mathcal{L}^0_{\mathrm{QCD}}$ is invariant under the global symmetry[2]

$$\mathrm{G}_\chi = \mathrm{SU}(3)_L \times \mathrm{SU}(3)_R \times \mathrm{U}(1)_V, \tag{1.26}$$

with $\mathrm{U}(1)_V = \mathrm{U}(1)_{L+R}$. The part $\mathrm{SU}(3)_L \times \mathrm{SU}(3)_R$ is known as chiral symmetry.

1.2.3 Explicit Symmetry Breaking

In QCD chiral symmetry arises when quark masses are zero. If we add the mass term,

$$-\bar{q}\,\mathcal{M}\,q = -\left(\bar{q}_L\,\mathcal{M}\,q_R + \bar{q}_R\,\mathcal{M}^\dagger\,q_L\right), \tag{1.27}$$

we observe that the chiral components of quark fields are mixed. The QCD Lagrangian is not invariant under the transformations (1.19) and chiral symmetry is explicitly broken. However, the breaking is small and $-\bar{q}\,\mathcal{M}\,q$ can be viewed as a perturbation. Hence, $\mathcal{L}_{\mathrm{QCD}}$ exhibits an approximate chiral symmetry at low energies.

[2]For completeness, we keep the part $\mathrm{U}(1)_V$ which could be omitted for the purposes of this work.

As chiral symmetry is approximate one can still rely on the Noether Theorem [71]. Then, the currents (1.23) provide the divergences,

$$\partial_\mu V^\mu_a = i\bar{q}\left[\mathcal{M}, \frac{\lambda_a}{2}\right] q \qquad \partial_\mu A^\mu_a = i\bar{q}\left\{\mathcal{M}, \frac{\lambda_a}{2}\right\} \gamma_5 q \tag{1.28a}$$

$$\partial_\mu V^\mu = 0 \qquad \partial_\mu A^\mu = 2i\, \bar{q}\,\mathcal{M}\gamma_5\, q + \frac{3g^2}{2(4\pi)^2}\,\epsilon_{\mu\nu\rho\sigma} G^{\mu\nu}_a G^{\rho\sigma}_a . \tag{1.28b}$$

Apart from $\partial_\mu V^\mu$ the divergences are non-zero. In general, the currents are not exactly conserved. They are broken by quark masses. The singlet axialvector current A^μ is broken by the term $2i\bar{q}\,\mathcal{M}\gamma_5\, q$ as well as by the anomaly. The multiplet currents A^μ_a are broken by a non-zero anticommutator. These currents are always not conserved if the mass term $-\bar{q}\,\mathcal{M}\,q$ is added. In general, the multliplet vector currents V^μ_a is also broken. The commutator in Eq. (1.28a) does not vanish unless $m_u = m_d = m_s$. In this case, V^μ_a is conserved and $\mathcal{L}_{\text{QCD}}$ is invariant under the transformations

$$\begin{aligned} q_L &\mapsto \mathcal{U}_V\, q_L \\ q_R &\mapsto \mathcal{U}_V\, q_R \end{aligned} \qquad \text{where} \qquad \mathcal{U}_V = \exp\left(-i\,\Theta^V_a \frac{\lambda_a}{2}\right) \in \mathrm{SU}(3)_V . \tag{1.29}$$

Here, Θ^V_a are eight real constant parameters. This invariance corresponds to the vector symmetry $\mathrm{SU}(3)_V = \mathrm{SU}(3)_{L+R}$. Note that the singlet vector current V^μ stays always conserved. It originates from a part of the symmetry (1.26) that is not broken by $\bar{q}\,\mathcal{M}\,q$. This part corresponds to $\mathrm{U}(1)_V$, namely to the transformations where q_L, q_R are rotated by the same phase factor.

We distinguish among four cases depending on the values of quark masses, see Ref. [62].

1. If $m_u = m_d = m_s = 0$, the currents V^μ_a, A^μ_a, V^μ are conserved. The singlet axialvector current A^μ has an anomaly and is not conserved. The Lagrangian $\mathcal{L}_{\text{QCD}}$ is invariant under $\mathrm{G}_\chi = \mathrm{SU}(3)_L \times \mathrm{SU}(3)_R \times \mathrm{U}(1)_V$ and hence, under chiral symmetry. The limit of zero masses is called chiral limit.

2. For mutually different quark masses one can rotate the chiral components of each flavors with the same phase factor. The Lagrangian $\mathcal{L}_{\text{QCD}}$ is invariant under the direct product $\prod_{f=1}^{3} \mathrm{U}(1)_f$. The single flavor currents $\bar{u}\gamma^\mu u$, $\bar{d}\gamma^\mu d$ and $\bar{s}\gamma^\mu s$ are conserved. Since the sum of such currents equals V^μ, the singlet vector current is conserved. In turn, the charge Q^V is a conserved quantity: it represents the difference of the number of quarks and antiquarks contained in a particle. This difference is commonly normalized to $B = Q^V/3$ and then, called baryon number. For mutually different quark masses the currents V^μ_a, A^μ_a, A^μ are not conserved.

3. If $m_u = m_d = m_s \neq 0$ the Lagrangian $\mathcal{L}_{\text{QCD}}$ is invariant under $\mathrm{SU}(3)_V \times \mathrm{U}(1)_V$ and hence, under the vector symmetry. The multiplet vector currents V^μ_a (as well as the singlet vector current V^μ) are conserved. Axialvector currents are not conserved. In this case, the divergence $\partial_\mu A^\mu_a$ has a particular structure: it is proportional to a pseudoscalar bilinear form containing the matrix λ_a.

4. If $m_u = m_d \neq m_s \neq 0$ the Lagrangian $\mathcal{L}_{\text{QCD}}$ is invariant under $\text{SU}(2)_V \times \text{U}(1)_V$. This is case of the isospin symmetry $\text{SU}(2)_V$ where u, d can be rotated into each others leaving the theory invariant. The u-quark represents a state with the isospin quantum number $I = 1/2$ and $I_3 = 1/2$ while the d-quark one with $I = 1/2$ and $I_3 = -1/2$. The isospin symmetry is more exactly realized than the vector symmetry as the difference $|m_d - m_u|$ is signicantly smaller than $|m_s - m_u|$ or $|m_s - m_d|$, see Tab. 1.1. The limit where $m_u = m_d \mathrel{\widehat{=}} \hat{m}$ is called isospin limit.

1.2.4 Spontaneous Symmetry Breaking and Goldstone Bosons

From previous considerations we would expect that hadrons are approximately grouped according to the irreducible representation of $\text{G}_\chi = \text{SU}(3)_L \times \text{SU}(3)_R \times \text{U}(1)_V$. Actually, $\text{U}(1)_V$ induces a grouping principle: depending on the value of the baryon number B, hadrons are grouped in mesons ($B = 0$) and baryons ($B = 1$). If the charges Q_a^A are generators of G_χ and commute with the QCD Hamiltonian, one would expect that each hadron state of a given parity is accompanied by a state with the opposite parity. This parity doubling is not present in the hadron spectrum, see Fig. 1.1. Rather than multiplets of opposite parity, hadrons are approximately grouped according to irreducible representations of SU(3) with one definite parity, see Ref. [76]. Moreover, the pseudoscalar mesons $\{\pi, K, \eta\}$ have remarkably small masses. They are spinless and are approximately grouped in an octet with a negative parity, see Tab. 1.2. These features suggest that chiral symmetry undergoes spontaneous symmetry breaking [77–79].

Spontaneous symmetry breaking (SSB) occurs whenever the ground state of a physical system is not fully invariant under the continuous symmetry of the theory. The symmetry is realized but does not appear in the ground state. It is hidden. A classical example is a ball on the top of a mexican hat. The system is rotation invariant with respect to the axis passing through the center of the ball and the top of the hat. The ball is not stable and will fall in a ground state within the hat brim. The fall occurs in a specific direction and the resulting ground state is not rotation invariant.

In general, SSB occurs if the Lagrangian is invariant under a continuous group G and the ground state is only invariant under a subgroup $\text{H} \subset \text{G}$. The group G has n_G generators and the subgroup has n_H generators. The generators of the subgroup annihilate the ground state. Each of them is associated to a massive state that is grouped in a n_H-multiplet according to the irreducible representation of H. The remaining $n_\text{GB} = n_\text{G} - n_\text{H}$ generators do not annihilate the ground state. They span a coset space G/H of order n_GB. The Goldstone Theorem [81, 82] asserts that each generator of the coset space is associated to a massless, spinless state called Goldstone boson. The Goldstone bosons have the symmetry properties of the generators of the coset space and are grouped in a n_GB-multiplet. They do not interact at rest because the strength of their interaction is proportional to their momenta. Note that the situation changes in presence of explicit symmetry breaking. If the breaking is small one can still rely on the Goldstone Theorem [81, 82] and Goldstone bosons acquire small masses proportional to the breaking parameter. In this case, the n_GB-multiplet is just approximate and Goldstone bosons slightly interact at rest.

Table 1.2: Flavor contents $q_f\bar{q}_{f'}$, masses M^{phys} and some quantum numbers of pseudoscalar mesons from Particle Data Group [2].

		$q_f\bar{q}_{f'}$	M^{phys} [MeV]	Q_e [e]	I	I_3	S
Pions	π^0	$\frac{1}{\sqrt{2}}(u\bar{u}-d\bar{d})$	134.9766 ± 0.0006	0	1	0	0
	π^+	$u\bar{d}$	139.57018 ± 0.00035	$+1$	1	$+1$	0
	π^-	$d\bar{u}$	139.57018 ± 0.00035	-1	1	-1	0
Kaons	K^+	$u\bar{s}$	493.677 ± 0.016	$+1$	$\frac{1}{2}$	$+\frac{1}{2}$	$+1$
	K^-	$s\bar{u}$	493.677 ± 0.016	-1	$\frac{1}{2}$	$-\frac{1}{2}$	-1
	K^0	$d\bar{s}$	497.614 ± 0.024	0	$\frac{1}{2}$	$-\frac{1}{2}$	$+1$
	$\bar{K}^0$	$s\bar{d}$	497.614 ± 0.024	0	$\frac{1}{2}$	$+\frac{1}{2}$	-1
Eta meson	η	$\frac{1}{\sqrt{6}}(u\bar{u}+d\bar{d}-2s\bar{s})$	547.862 ± 0.018	0	0	0	0

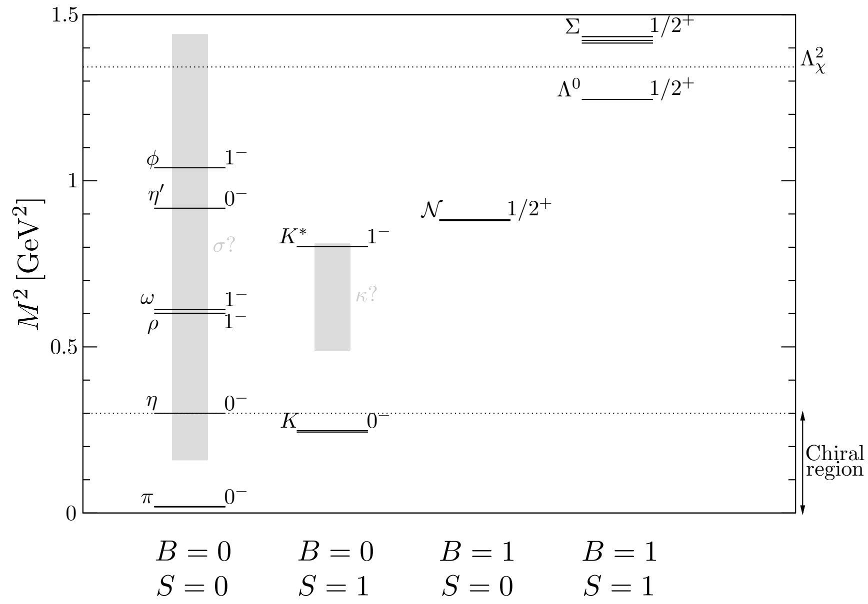


Figure 1.1: Hadron spectrum taken from [80]. Hadron states are represented depending on the value of the baryon number B and of the strangeness quantum number S. For each hadron is additionally displayed J^P i.e. the value of the total angular momentum J and of the parity P.

Let us apply these general considerations to the group $\mathrm{G}_\chi = \mathrm{SU}(3)_L \times \mathrm{SU}(3)_R \times \mathrm{U}(1)_V$. We assume that the subgroup $\mathrm{H}_\chi = \mathrm{SU}(3)_V \times \mathrm{U}(1)_V$ leaves the ground state invariant. The generators Q_a^A do not annihilate the ground state and span the coset space $\mathrm{G}_\chi/\mathrm{H}_\chi$. By virtue of the Goldstone Theorem [81,82] each generator of the coset space is associated to a spinless Goldstone boson which in presence of explicit symmetry breaking acquires a small mass. The Goldstone bosons have negative parity and are grouped in an octet according to the irreducible representation of H_χ. In the hadron spectrum the pseudoscalar mesons $\{\pi, K, \eta\}$ have similar properties: they are spinless, have small masses, negative parity and are grouped in an approximate octet. Hence, $\{\pi, K, \eta\}$ can be identified with the eight Goldstone bosons arising from spontaneous breaking of $\mathrm{SU}(3)_L \times \mathrm{SU}(3)_R \times \mathrm{U}(1)_V$ down to $\mathrm{SU}(3)_V \times \mathrm{U}(1)_V$.

A series of theoretical arguments confirm that chiral symmetry undergoes such SSB. In Ref. [83] Coleman and Witten show under reasonable assumptions that for $N_\mathrm{c} \to \infty$ where N_c is the number of colors, the symmetry $\mathrm{U}(N_\mathrm{f})_L \times \mathrm{U}(N_\mathrm{f})_R$ is either exact or is spontaneously broken down to $\mathrm{SU}(N_\mathrm{f})_V \times \mathrm{U}(1)_V$. The authors then exclude the first case applying a method of 't Hooft [84] based on the anomaly of Adler, Bell, Jackiw [72, 75]. In Ref. [85] Vafa and Witten show under plausible assumptions that in a vector-like gauge theory like QCD, the vector part of chiral symmetry is not spontaneously broken. This means that the subgroup $\mathrm{SU}(3)_V \times \mathrm{U}(1)_V$ does not break spontaneously. Furthermore, recent simulations of Lattice QCD confirm a non-zero quark condensate in chiral limit: $\langle u\bar{u}\rangle = -(271 \pm 15\ \mathrm{MeV})^3$, see Ref. [86–89]. Such result implies the existence of the massless states required by the Goldstone Theorem and can only occur if chiral symmetry is spontaneously broken [90].

One can show that there is a map from the coset space $\mathrm{G}_\chi/\mathrm{H}_\chi$ into the vector space of the fields of Goldstone bosons, see Ref. [62, 91, 92]. The map is surjective as well as injective and allows one to express the fields of Goldstone bosons in a 3×3 unitary matrix,

$$U(x) = \exp\left(i\,\frac{\Phi(x)}{F_0} \right). \tag{1.30}$$

Here, $\Phi(x)$ contains the fields of Goldstone bosons and is an hermitian matrix,

$$\begin{aligned}
\Phi(x) = \lambda_a \phi_a(x) &= \begin{pmatrix} \phi_3 + \frac{1}{\sqrt{3}}\phi_8 & \phi_1 - i\phi_2 & \phi_4 - i\phi_5 \\ \phi_1 + i\phi_2 & -\phi_3 + \frac{1}{\sqrt{3}}\phi_8 & \phi_6 - i\phi_7 \\ \phi_4 + i\phi_5 & \phi_6 + i\phi_7 & -\frac{2}{\sqrt{3}}\phi_8 \end{pmatrix} \\
&= \begin{pmatrix} \pi^0 + \frac{1}{\sqrt{3}}\eta & \sqrt{2}\pi^+ & \sqrt{2}K^+ \\ \sqrt{2}\pi^- & -\pi^0 + \frac{1}{\sqrt{3}}\eta & \sqrt{2}K^0 \\ \sqrt{2}K^- & \sqrt{2}\bar{K}^0 & -\frac{2}{\sqrt{3}}\eta \end{pmatrix}.
\end{aligned} \tag{1.31}$$

The parameter F_0 is the decay constant in chiral limit and is defined by the matrix elements of the axialvector decay of Goldstone bosons,

$$\langle 0|\, A_a^\mu(x)\, |\phi_b(p)\rangle = i\, p^\mu\, \delta_{ab} F_0\, \mathrm{e}^{-ipx}. \tag{1.32}$$

In a first approximation, F_0 can be equaled to the decay constant of pions whose value is measured experimentally [2]:

$$F_\pi = F_0\, [1 + \mathcal{O}(m_f)] = (92.2 \pm 0.01)\ \mathrm{MeV}. \tag{1.33}$$

However, keep in mind that F_0 is a parameter of the strong interaction since pions do not decay in QCD (nor in massless QCD) until one accounts for the weak interaction. From the matrix elements (1.32) we can see that Goldstone bosons are indeed massless states. Deriving both sides of the equation, we obtain

$$\partial_\mu \langle 0|\, A_a^\mu(x)\, |\phi_b(p)\rangle = p^2\, \delta_{ab} F_0\, \mathrm{e}^{-ipx}. \tag{1.34}$$

As the multiplet axialvector currents are conserved in chiral limit, the left-hand side of the equation vanishes. This implies that the momentum square p^2 on the right-hand side must also vanish and that $|\phi_b\rangle$ are massless states, as expected for Goldstone bosons.

We return to the unitary matrix (1.30) and to the bijective map from $\mathrm{G}_\chi/\mathrm{H}_\chi$ into the vector space of the fields of Goldstone bosons. As the set of unitary matrices does not define a vector space (the sum of two unitary matrices does not give a unitary matrix) the map is not a representation but rather a non-linear realization. The unitary matrix $U(x)$ transforms under $\mathrm{SU}(3)_L \times \mathrm{SU}(3)_R$ as

$$U(x) \mapsto \mathcal{U}_R\, U(x)\, \mathcal{U}_L^\dagger \qquad \text{where} \qquad \begin{array}{l} \mathcal{U}_L \in \mathrm{SU}(3)_L \\ \mathcal{U}_R \in \mathrm{SU}(3)_R. \end{array} \tag{1.35}$$

The ground state corresponds to $U(x) = U_0 = \mathbb{1}_3$ [or $\Phi(x) = 0$] and is invariant under $\mathrm{SU}(3)_V$. This can be easily showed if we consider transformations that rotate the chiral components in the same way, see Eq. (1.29). Setting $\mathcal{U}_V = \mathcal{U}_L = \mathcal{U}_R$ in (1.35) we obtain

$$U_0 \mapsto \mathcal{U}_V\, U_0\, \mathcal{U}_V^\dagger = \mathcal{U}_V\, \mathcal{U}_V^\dagger = \mathbb{1}_3 = U_0. \tag{1.36}$$

If we take transformations that rotate the left chiral component by $\mathcal{U}_A$ and the right chiral component by $\mathcal{U}_A^\dagger$ the ground state does not remain invariant,

$$U_0 \mapsto \mathcal{U}_A^\dagger\, U_0\, \mathcal{U}_A^\dagger = \mathcal{U}_A^\dagger\, \mathcal{U}_A^\dagger \neq U_0. \tag{1.37}$$

This is in agreement with spontaneous symmetry breaking of chiral symmetry.

1.2.5 QCD with External Fields and the Generating Functional

We couple external fields to the massless theory and introduce the generating functional. This allows us to express Green functions as well as their symmetry relations (i.e. chiral Ward identities) in a very concise way. Green functions are expressed as functional derivatives of the generating functional and chiral Ward identities are equivalent (in the absence of anomalies) to the invariance of the latter under local transformations of external fields, see Ref. [58]. There is another practical advantage: external fields allow us to introduce electromagnetic and weak interactions. For the purpose of this work, we outline the case of the electromagnetic interaction.

We consider the evolution of massless QCD in the presence of external fields v^μ, a^μ, s and p. In the remote past the system is in the initial ground state $|0_{\text{in}}\rangle_{v,a,s,p}$. Far in the future the system ends in the ground state $\langle 0_{\text{out}}|$. The generating functional represents the probability amplitude for the transition of the system, from the initial state to the final one, in the presence of external fields,

$$\mathrm{e}^{i\,Z[v,a,s,p]} = \langle 0_{\text{out}}\,|\,0_{\text{in}}\rangle_{v,a,s,p} = \langle 0|\,T\left\{\mathrm{e}^{i\int \mathrm{d}^4x\,\mathcal{L}_{\text{ext}}(x)}\right\}|0\rangle\,. \tag{1.38}$$

The operator T is the time-ordering operator and $\mathcal{L}_{\text{ext}}$ is the part of the Lagrangian containing the external fields,

$$\mathcal{L} = \mathcal{L}^0_{\text{QCD}} + \mathcal{L}_{\text{ext}} = \mathcal{L}^0_{\text{QCD}} + \bar{q}\gamma^\mu\left(v_\mu + \gamma_5 a_\mu\right)q - \bar{q}\,(s - ip)\,q. \tag{1.39}$$

The external fields v^μ, a^μ, s, p are color neutral objects. They are hermitian matrices in flavor space and can be expressed in terms of Gell-Mann matrices,

$$\begin{aligned} v^\mu &= \frac{\lambda_0}{\sqrt{6}}\,v_0^\mu(x) + \frac{\lambda_b}{2}\,v_b^\mu(x) \qquad & s &= \lambda_0\,s_0(x) + \lambda_b\,s_b(x) \\ a^\mu &= \frac{\lambda_b}{2}\,a_b^\mu(x) & p &= \lambda_0\,p_0(x) + \lambda_b\,p_b(x). \end{aligned} \tag{1.40}$$

Here, the repetition of the index implies sums over $b = 1, \ldots, 8$ and $\lambda_0 = \sqrt{2/3}\,\mathbb{1}_3$. The field v_0^μ couple to the singlet vector current V^μ whereas the fields v_b^μ (resp. a_b^μ) couple to the multiplet vector currents V_b^μ (resp. multiplet axialvector currents A_b^μ). The fields s_0, s_b (resp. p_0, p_b) couple to scalar densities (resp. pseudoscalar densities),

$$\begin{aligned} S_0 &= \bar{q}\lambda_0\,q \qquad & P_0 &= i\,\bar{q}\,\gamma_5\lambda_0\,q \\ S_b &= \bar{q}\,\lambda_b\,q & P_b &= i\,\bar{q}\,\gamma_5\lambda_b\,q. \end{aligned} \tag{1.41}$$

Note that for $v^\mu = a^\mu = p = 0$ and $s = \mathcal{M}$ the Lagrangian $\mathcal{L}$ reduces to the QCD Lagrangian of Eq. (1.14). In that case, $\mathcal{L}_{\text{ext}}$ corresponds to the mass term $-\bar{q}\,\mathcal{M}\,q$.

The Lagrangian $\mathcal{L}$ is hermitian and invariant under charge-conjugation, parity, time reversal transformations. This means that v^μ, a^μ, s, p transform like: vector, axialvector, scalar and pseudoscalar fields, respectively. Furthermore, $\mathcal{L}$ is invariant under the local transformations,

$$
\begin{aligned}
q_L &\mapsto \mathrm{e}^{-i\,\frac{\Theta(x)}{3}}\,\mathcal{U}_L(x)\,q_L \qquad && \mathcal{U}_L(x) \in \mathrm{SU}(3)_L \\
q_R &\mapsto \mathrm{e}^{-i\,\frac{\Theta(x)}{3}}\,\mathcal{U}_R(x)\,q_R \qquad && \mathcal{U}_R(x) \in \mathrm{SU}(3)_R .
\end{aligned}
\tag{1.42}
$$

Here, $\Theta(x)$ is the real function which parametrizes local transformations $\mathrm{e}^{-i\,\frac{\Theta(x)}{3}} \in \mathrm{U}(1)_V$. The invariance of the Lagrangian under the local transformations (1.42) implies that external fields transform like gauge fields,

$$
\begin{aligned}
(v^\mu - a^\mu) &\mapsto \mathcal{U}_L(x)(v^\mu - a^\mu)\,\mathcal{U}_L^\dagger(x) + i\,\mathcal{U}_L(x)\,\partial^\mu \mathcal{U}_L^\dagger(x) - \partial^\mu\Theta(x) \\
(v^\mu + a^\mu) &\mapsto \mathcal{U}_R(x)(v^\mu + a^\mu)\,\mathcal{U}_R^\dagger(x) + i\,\mathcal{U}_R(x)\,\partial^\mu \mathcal{U}_R^\dagger(x) - \partial^\mu\Theta(x) \\
(s - i\,p) &\mapsto \mathcal{U}_R(x)(s - i\,p)\,\mathcal{U}_L^\dagger(x) \\
(s + i\,p) &\mapsto \mathcal{U}_L(x)(s + i\,p)\,\mathcal{U}_R^\dagger(x).
\end{aligned}
\tag{1.43}
$$

The generating functional collects Green functions formed by the symmetry currents and densities. Green functions can be obtained through functional derivatives with respect to v^μ, a^μ, s, p. Chiral Ward identities are automatically satisfied due to the invariance of the generating functional under the local transformations (1.43). Green functions of QCD can be obtained evaluating at $v^\mu = a^\mu = p = 0$ and $s = \mathcal{M}$.

We can introduce electromagnetic and weak interactions considering external fields as gauge fields. For instance, the electromagnetic interaction can be introduced through the vector field,

$$
v^\mu = -eA^\mu(x)\,\mathcal{Q}. \tag{1.44}
$$

Here, e is the elementary electric charge, $A^\mu(x)$ is the electromagnetic gauge field and $\mathcal{Q} = \mathrm{diag}(2/3, -1/3, -1/3)$ is the matrix with the electric charges of quarks in elementary units. In this case, $\mathcal{L}_{\text{ext}}$ corresponds to $-e\,\bar{q}\,\gamma^\mu A_\mu(x)\mathcal{Q}\,q - \bar{q}\,\mathcal{M}\,q$ if $a^\mu = p = 0$, $s = \mathcal{M}$ and the electromagnetic Ward identities are automatically satisfied as v^μ transforms as a gauge field.

In the above discussion, we have intentionally omitted the field coupling to the singlet axialvector current and deliberately ignored the anomaly. It is possible to include the anomaly by adding an appropriate term. In Ref. [93, 94] Wess, Zumino and Witten construct a generating functional which includes the anomaly in the so-called Wess–Zumino–Witten term. This term successfully describes specific physical processes, such as the decay of the neutral pion into two photons: $\pi^0 \to \gamma\gamma$, see Ref. [62, 94].

1.3 Effective Chiral Lagrangian

1.3.1 Construction

We are now in position to construct the effective Lagrangian of ChPT. In Section 1.1 we have seen that the Weinberg Theorem [9] provides the general principles to construct the effective Lagrangian: one writes down all possible terms containing the fields of active particles which are allowed by the symmetry of the underlying fundamental theory. The symmetry just provides the structure of the terms but not the strength of their coupling constants. These are encoded in a set of low-energy constants (LEC) that represent the free parameters of the EFT. In ChPT, the LEC must be determined either by the comparison with phenomenology or by the direct calculation in Lattice QCD.

There are infinitely many terms containing the fields of Goldstone bosons which are allowed by chiral symmetry. If we then promote chiral symmetry to a local symmetry, terms containing external fields are allowed as well. In principle, once one term is found, each power of it is a possible candidate. It is convenient to introduce a scheme that orders the terms of the effective Lagrangian by means of their relevance. In ChPT, one usually adopts the Weinberg counting scheme [9] which orders the terms in powers of momenta. The counting rules are

$$\begin{array}{rcc} U \sim \mathcal{O}(p^0) & & \\ \partial^\mu U \sim \mathcal{O}(p^1) & v^\mu, a^\mu \sim \mathcal{O}(p^1) & \\ \partial^\mu \partial^\nu U \sim \mathcal{O}(p^2) & \partial^\nu v^\mu, \partial^\nu a^\mu \sim \mathcal{O}(p^2) & s, p \sim \mathcal{O}(p^2) \\ \vdots & \vdots & \vdots \end{array} \tag{1.45}$$

The first rule indicates that the unitary matrix $U = U(x)$ counts as a constant like the ground state, $U_0 = \mathbb{1}_3$. Successive rules indicate that each derivative ∂^μ counts as a power of a momentum like in Fourier space. The external fields v^μ, a^μ count as $\mathcal{O}(p^1)$ because they are at the same level of ∂^μ. The fields s, p count as the square of a momentum $\mathcal{O}(p^2)$ as we will see in Section 1.4.1. By means of these rules, the effective Lagrangian can be ordered as a series in powers of momenta where odd powers are excluded due to Lorentz invariance,

$$\mathcal{L}_{\text{eff}} = \mathcal{L}_2 + \mathcal{L}_4 + \mathcal{L}_6 + \ldots \tag{1.46}$$

Note that $\mathcal{L}_0$ is excluded by the unitarity (viz. $U^\dagger U = \mathbb{1}_3$): such term would be an irrelevant constant reflecting the fact that Goldstone bosons do not interact at rest.

At leading order $\mathcal{O}(p^2)$ there are only two terms allowed by the local chiral symmetry. These were found in Ref. [95–97] after having worked out the linear σ-model [98–100], see also Ref. [9, 57] and review articles cited therein. In the notation of Gasser and Leutwyler [11] they read

$$\mathcal{L}_2 = \frac{F_0^2}{4} \langle D_\mu U \, (D^\mu U)^\dagger + \chi U^\dagger + U \chi^\dagger \rangle \,. \tag{1.47}$$

Here, $\langle\,.\,\rangle$ is the trace in flavor space and F_0 is the parameter of Eq. (1.32). The prefactor $F_0^2/4$ is chosen so that $\mathcal{L}_2$ reduces to the usual kinetic term (i.e. $\frac{1}{2}\partial_\mu\phi_a\partial^\mu\phi_a$) if one sets $v^\mu = a^\mu = s = p = 0$ and expands the unitary matrix as

$$U = \mathbb{1}_3 + i\,\frac{\Phi}{F_0} - \frac{\Phi^2}{2F_0^2} + \mathcal{O}(\Phi^3). \tag{1.48}$$

The covariant derivative $D^\mu U$ is defined so that under the local transformations (1.42) it transforms in the same way as the unitary matrix U,

$$D^\mu U \mapsto \mathcal{U}_R(x)\, D^\mu U\, \mathcal{U}_L^\dagger(x) \qquad \text{with} \qquad \begin{array}{l} \mathcal{U}_L(x) \in \mathrm{SU}(3)_L \\ \mathcal{U}_R(x) \in \mathrm{SU}(3)_R. \end{array} \tag{1.49}$$

This request introduces vector and axiavector fields by means of the minimal coupling prescription,

$$D^\mu U = \partial^\mu U - i\,[v^\mu, U] - i\,\{a^\mu, U\}\,. \tag{1.50}$$

The matrix χ contains scalar and pseudoscalar fields,

$$\chi = 2B_0\,(s + i\,p)\,, \tag{1.51}$$

and transforms as $\chi \mapsto \mathcal{U}_R(x)\,\chi\,\mathcal{U}_L^\dagger(x)$ as a result of Eq. (1.43). Note that B_0 is a free parameter like F_0: they represent the LEC at $\mathcal{O}(p^2)$ and are related to the quark condensate of QCD as $F_0^2 B_0 = -\langle u\bar{u}\rangle$, see Ref. [62].

At successive orders the number of terms allowed by local chiral symmetry rapidly increase. The reason is, each product resulting from two terms $\mathcal{O}(p^2)$ is a possible candidate. Moreover, new terms are allowed by the symmetry. At next-to-leading order (NLO) there are twelve terms allowed by the local chiral symmetry. They were found out by Gasser and Leutwyler in Ref. [11] and can be summarized as

$$\mathcal{L}_4 = \sum_{j=1}^{12} L_j P_j. \tag{1.52}$$

Here, P_j are monomials containing U, external fields and derivatives thereof. The first ten monomials $P_1, \ldots, P_{10}$ describe physical processes; the last two monomials P_{11}, P_{12} contain just external fields and hence, do not describe physical processes. The coupling constants $L_1, \ldots, L_{12}$ are not determined by the symmetry and their finite values represent the LEC at $\mathcal{O}(p^4)$.

At next-to-next-to-leading order (NNLO) the effective Lagrangian is composed by even more terms [101–105]. The simplest version involves 94 terms, see Ref. [102]. The construction proceeds as for $\mathcal{L}_2$, $\mathcal{L}_4$ but is complicated due to the large number of terms, one must account for. Another complication is to determine the minimal set of independent terms and rule out redundant structures. To-date there is no systematic method to determine independent terms. The accumulated experience just confirms that the number of redundant structures is decreased during years. Recently, another term was ruled out from the version of $\mathcal{L}_6$ with 2 light flavors, see Ref. [106]. Despite these complications many physical quantities are known up to $\mathcal{O}(p^6)$: for an overview we direct to Ref. [107].

1.3.2 Path-Integral Representation of the Generating Functional

In Section 1.2.5 we introduce the generating functional for an extended version of QCD. At low energies, the generating functional can be represented by the path integral

$$\mathrm{e}^{i\, Z_{\text{eff}}[v,a,s,p]} = \int [\,\mathrm{d}\, U(\Phi)]\, \mathrm{e}^{i \int \mathrm{d}^4x\, \mathcal{L}_{\text{eff}}}. \tag{1.53}$$

By construction, the effective Lagrangian $\mathcal{L}_{\text{eff}}$ is invariant under the local chiral symmetry and includes the external fields v^μ, a^μ, s, p. The effective Lagrangian can be expanded in even powers of momenta and such expansion induces an analogous one for the functional $Z_{\text{eff}} = Z_{\text{eff}}\,[v, a, s, p]$:

$$Z_{\text{eff}} = Z_2 + Z_4 + \dots \tag{1.54}$$

The terms are ordered according to the Weinberg counting scheme [9]. Note that the scheme also orders Feynman diagrams in terms of the chiral order D. A diagram with N_L loops and N_{2n} vertices from $\mathcal{L}_{2n}$ counts as $\mathcal{O}(p^D)$ where

$$D = 2\,(N_L + 1) + \sum_{n\geq 1} 2\,(n-1)\,N_{2n}. \tag{1.55}$$

hs has non-negative terms since the effective Lagrangian starts with $n = 1$. This formula allows us to distinguish the terms of the functional Z_{eff} by means of the chiral order and identify the Feynman diagrams which contribute. Up to $\mathcal{O}(p^4)$ we have,

$$\begin{aligned}
&D = 2: \quad N_L = 0, \quad n = 1 && Z_2 = \textstyle\int \mathrm{d}^4x\, \mathcal{L}_2 \\
&D = 4: \quad N_L = 0, \quad n = 2 && Z_4^{N_L=0} = \textstyle\int \mathrm{d}^4x\, \mathcal{L}_4 + Z_{\text{WZW}} \\
& N_L = 1, \quad n = 1 && Z_4^{N_L=1} \text{ with vertices of } \mathcal{L}_2.
\end{aligned} \tag{1.56}$$

At leading order, Z_{eff} coincides with Z_2, namely with the classical action $\int \mathrm{d}^4x\, \mathcal{L}_2$. This term incorporates the contributions of tree graphs (i.e. $N_L = 0$) with vertices of $\mathcal{L}_2$ (i.e. $n = 1$). At NLO the functional consists of two subterms: $Z_4 = Z_4^{N_L=0} + Z_4^{N_L=1}$. The subterm $Z_4^{N_L=0}$ incorporates the contributions of tree graphs ($N_L = 0$) with vertices of $\mathcal{L}_4$ (i.e. $n = 2$) while $Z_4^{N_L=1}$ incorporates the contributions of one-loop diagrams ($N_L = 1$) with vertices of $\mathcal{L}_2$. Acutally, the subterm $Z_4^{N_L=0}$ consists of the action $\int \mathrm{d}^4x\, \mathcal{L}_4$ plus the Wess–Zumino–Witten term Z_{WZW}. Here, we have added Z_{WZW} only to show where it enters in the path-integral representation of the generating functional. This describes processes with odd intrinsic parity involving an odd number of pseudoscalar mesons. Since here we are not interessed on such processes we can ignore Z_{WZW} for the remainder.

According to the formula (1.55) loop diagrams start at $\mathcal{O}(p^4)$. Their contributions are divergent and must be renormalized. To treat divergences we choose a regularization scheme that is independent from masses and at the same time, respects the symmetry properties of the effective Lagrangian. A possible choice is dimensional regularization which treats divergences by means of a d-dimensional space-time. As $\mathcal{L}_{\text{eff}}$ is the most general effective Lagrangian allowed by the local chiral symmetry, it already contains all counterterms needed for the renormalization, see Ref. [108]. Then, the renormalization absorbs the divergences through the redefinition of the coupling constants. This occurs at each order of the chiral expansion (1.54) so that Z_{eff} is renormalized order by order.

We briefly illustrate the renormalization of Z_4. At $\mathcal{O}(p^4)$ the divergences arise from one-loop diagrams and are incorporated in $Z_4^{N_L=1}$. According to Ref. [108] such divergences have the form of an action with the symmetry properties of $\mathcal{L}_2$. They could be expressed in a Lagrangian of the form [109]

$$\mathcal{L}_{4,\text{div}}^{N_L=1} = -\lambda(\mu) \sum_{j=1}^{12} \Gamma_j P_j, \tag{1.57}$$

where P_j coincide with the monomials of Eq. (1.52) and Γ_j are rational numbers, see Ref. [11]. The precise expression of $\lambda(\mu)$ depends on the regularization scheme and in our case[3] reads

$$\lambda(\mu) = \frac{\mu^{d-4}}{2(4\pi)^2} \Big\{ \frac{2}{d-4} - \big[\ln(4\pi) + \Gamma'(1) + 1 \big] \Big\}. \tag{1.58}$$

Here, μ is the renormalization scale and $\Gamma'(1)$ is the derivative of Gamma function $\Gamma(z)$ at $z = 1$. Note that divergences appear as simple poles if $d \to 4$. To renormalize Z_4 we redefine the coupling constants of $Z_4^{N_L=0}$ that are contained in the action $\int \mathrm{d}^4 x\, \mathcal{L}_4$:

$$L_j = L_j^{\text{r}}(\mu) + \Gamma_j \lambda(\mu), \qquad j = 1, \ldots, 12. \tag{1.59}$$

The renormalized LEC $L_j^{\text{r}}(\mu)$ correspond to the finite parts of the coupling constants of Eq. (1.52). The redefinition absorbs the divergences (1.57) so that the sum,

$$Z_4^{N_L=1} + \int \mathrm{d}^4 x\, \mathcal{L}_4\left(L_i\right) = Z_{4,\text{fin}}^{N_L=1}\left(\mu\right) + \int \mathrm{d}^4 x\, \mathcal{L}_4\big(L_j^{\text{r}}(\mu)\big), \tag{1.60}$$

is finite on both sides of the equation. On the right-hand side, $Z_{4,\text{fin}}^{N_L=1}(\mu)$ incorporates the finite contributions of one-loop diagrams at $\mathcal{O}(p^4)$ and the action $\int \mathrm{d}^4 x\, \mathcal{L}_4\big(L_j^{\text{r}}(\mu)\big)$ contains renormalized LEC. Their dependence on the renormalization scale cancels out in all Green functions so that results of physical observables are finite and independent from μ.

1.3.3 Restriction to Two Light Flavors

If we study energies $E \ll 0.5$ GeV we can integrate out the degrees of freedom of the s-quark and consider $N_{\text{f}} = 2$ light flavors. The group is restricted to $\mathrm{G}_\chi = \mathrm{SU}(2)_L \times \mathrm{SU}(2)_R \times \mathrm{U}(1)_V$ and the pions –which in the hadron spectrum are approximately grouped as a triplet– can be identified with the three Goldstone bosons arising from the spontaneous breaking to $\mathrm{H}_\chi = \mathrm{SU}(2)_V \times \mathrm{U}(1)_V$. The formalism introduced so far remains mostly unchanged and

[3] We use dimensional regularization in the modified minimal subtraction ($\overline{\text{MS}} + 1$) scheme.

the necessary modifications can be included in a straightforward way. We just discuss the relevant modifications needed for this work. Further details can be found in Ref. [10].

The restriction of the group to two light flavors implies that at the place of Gell-Mann matrices we must use the generators of SU(2), namely Pauli matrices

$$\tau_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \tau_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \tau_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{1.61}$$

Then, v^μ, a^μ, s, p and $\Phi(x)$ are expressed in their terms and are 2×2 matrices in flavor space. For example,

$$\Phi(x) = \tau_a \phi_a = \begin{pmatrix} \phi_3 & \phi_1 - i\phi_2 \\ \phi_1 + i\phi_2 & -\phi_3 \end{pmatrix} = \begin{pmatrix} \pi^0 & \sqrt{2}\pi^+ \\ \sqrt{2}\pi^- & -\pi^0 \end{pmatrix}. \tag{1.62}$$

Here, the repetition of the index implies a sum over $a = 1, 2, 3$. The definitions (1.30, 1.50, 1.51) remain unchanged apart from the fact that U, $D^\mu U$, χ become 2×2 matrices, too.

In general, the form of the effective Lagrangian $\mathcal{L}_{\text{eff}}$ must be modified. Some structures are redundant and must be ruled out. At leading order, $\mathcal{L}_2$ has the same structures as in the 3-light-flavor case, see Eq. (1.47). Only, F_0, B_0 are replaced by

$$F = F_0 \left[1 + \mathcal{O}(m_s)\right] \qquad B = B_0 \left[1 + \mathcal{O}(m_s)\right]. \tag{1.63}$$

These new parameters encode information on the s-quark which is now treated as heavy. Hence, F, B have a different physical meaning compared to F_0, B_0.

At NLO the effective Lagrangian consists of ten terms. These were found by Gasser and Leutwyler in Ref. [10] and can be summarized as

$$\mathcal{L}_4 = \sum_{j=1}^{10} \ell_j P_j. \tag{1.64}$$

The monomials P_j are different from those of Eq. (1.52). Here, $P_1, \ldots, P_7$ describe physical processes. The last three monomials P_8, P_9, P_{10} contain just external fields and do not describe physical processes. The coupling constants $\ell_1, \ldots, \ell_{10}$ take the place of the 3-light-flavor constants L_j. They can be redefined and absorb the divergences at $\mathcal{O}(p^4)$. The redefinition reads

$$\ell_j = \ell_j^{\mathrm{r}}(\mu) + \gamma_j \lambda(\mu), \tag{1.65}$$

where $\ell_j^{\mathrm{r}}(\mu)$ are renormalized LEC and γ_j are rational numbers, see Ref. [10]. Often, the renormalized LEC $\ell_j^{\mathrm{r}}(\mu)$ are replaced by constants which are independent from the renormalization scale μ. The μ-dependence is isolated in a logarithm according to

$$\ell_j^{\mathrm{r}}(\mu) = \frac{\gamma_j}{2N}\left[\bar{\ell}_j + \log\left(\frac{M^2}{\mu^2}\right)\right], \tag{1.66}$$

where $M^2 = B(m_u + m_d)$ and $N = (4\pi)^2$. The constants $\bar{\ell}_j$ are μ-independent and were originally introduced in Ref. [10]. Note that in chiral limit (i.e. for $m_u, m_d \to 0$) the definition (1.66) is not valid and one can not use $\bar{\ell}_j$.

1.4 Applications of ChPT

We present some applications of ChPT up to $\mathcal{O}(p^4)$. We calculate masses, decay constants, pseudoscalar coupling constants and form factors. The results and the derivations presented will be extensively used in the rest of the work.

1.4.1 Masses

In ChPT the masses of pseudoscalar mesons are calculated setting $v^\mu = a^\mu = p = 0$, $s = \mathcal{M}$ in the functional Z_{eff}. At leading order the masses can be directly read from the classical action $\int \mathrm{d}^4x\, \mathcal{L}_2$. Inserting the expansion (1.48) in $\mathcal{L}_2$ and retaining terms $\mathcal{O}(\Phi^2)$ we obtain,

$$\begin{aligned} \mathring{M}_\pi^2 &= 2B_0\hat{m} \\ \mathring{M}_K^2 &= B_0\left(\hat{m} + m_s\right) \\ \mathring{M}_\eta^2 &= \frac{2}{3}B_0\left(\hat{m} + 2m_s\right). \end{aligned} \tag{1.67}$$

Note that from here on we set $m_u = m_d = \hat{m}$ and work in isospin limit. The above expressions correspond to Gell-Mann–Oakes–Renner formulae [110]. One can show that they satisfy the Gell-Mann–Okubo relation [76, 111, 112]:

$$4\mathring{M}_K^2 = 3\mathring{M}_\eta^2 + \mathring{M}_\pi^2. \tag{1.68}$$

As the expressions (1.67) are at leading order, the masses count as $\mathring{M}_\pi^2$, $\mathring{M}_K^2$, $\mathring{M}_\eta^2 \sim \mathcal{O}(p^2)$. This is in agreement with the on-shell condition $p^2 = M^2$. From the right-hand side of Eq. (1.67) follows that quark masses count as the square of a momentum. In turn, the mass matrix counts as $\mathcal{M} \sim \mathcal{O}(p^2)$. Since $s = \mathcal{M}$, we deduce that the external scalar field counts as $s \sim \mathcal{O}(p^2)$, too. This justifies the counting rule presented in Eq. (1.45).

In general, the mass of a particle is defined by the pole of the full propagator. For a pseudoscalar particle P, the full propagator reads

$$\frac{\Delta_P(p)}{i} = \frac{1}{i\left[\mathring{M}_P^2 - p^2 - \Sigma_P(p^2) - i\epsilon\right]}, \qquad \epsilon > 0. \tag{1.69}$$

Here, $\mathring{M}_P$ is the contribution to the mass at leading order and Σ_P is the self energy of P. The mass of the particle corresponds to the solution of the pole equation,

$$\mathring{M}_P^2 - p^2 - \Sigma_P(p^2) = 0, \qquad \text{for} \quad p^2 = M_P^2. \tag{1.70}$$

At NLO we can expand the self energy as

$$\Sigma_P(p^2) = A_P + B_P\, p^2 + \mathcal{O}(p^6), \tag{1.71}$$

(a) Tree graph. *(b) Tadpole diagram.*

Figure 1.2: Contributions to the self energies at NLO. Solid lines stand for pseudoscalar mesons. The square corresponds to a vertex of $\mathcal{L}_4$ whereas the intersection of four lines corresponds to a vertex of $\mathcal{L}_2$.

where the coefficients A_P, B_P count as $A_P \sim \mathcal{O}(p^4)$ resp. $B_P \sim \mathcal{O}(p^2)$. Inserting the expansion in Eq. (1.70) we obtain the mass of the particle,

$$\begin{aligned} M_P^2 &= \left[\mathring{M}_P^2 - A_P\right](1+B_P)^{-1} + \mathcal{O}(p^6) \\ &= \mathring{M}_P^2 - A_P - \mathring{M}_P^2 \, B_P + \mathcal{O}(p^6). \end{aligned} \tag{1.72}$$

We can now reexpress the full propagator in terms of the mass M_P as

$$\frac{\Delta_P(p)}{i} = \frac{Z_P}{i\left[M_P^2 - p^2 - i\epsilon\right]}, \tag{1.73}$$

where Z_P is the renormalization constant of the particle wavefunction at NLO, i.e.

$$Z_P = \frac{1}{1+B_P}. \tag{1.74}$$

In ChPT the self energies of pseudoscalar mesons have two contributions at NLO. They are represented by the diagrams of Fig. 1.2. The tree graph has a vertex of $\mathcal{L}_4$ in which two pseudoscalar mesons couple together. The contribution can be directly read from $\mathcal{L}_4$. The tadpole diagram has a vertex of $\mathcal{L}_2$ in which four pseudoscalar mesons couple together. Two lines are closed and form a loop. The loop can be evaluated integrating over all possible values, taken by the momentum flowing in the loop. Such integration leads to divergences that can be treated by means of dimensional regularization. Altogether, the diagrams of Fig. 1.2 contribute to the self energies of pseudoscalar mesons as

$$\begin{aligned} \Sigma_\pi &= A_\pi + B_\pi \, p^2 \\ \Sigma_K &= A_K + B_K \, p^2 \\ \Sigma_\eta &= A_\eta + B_\eta \, p^2, \end{aligned} \tag{1.75}$$

where the coefficients are

$$A_\pi = \frac{\overset{\circ}{M}{}_\pi^2}{F_0^2}\left\{\frac{\Delta_\pi}{6\,i} + \frac{\Delta_K}{3\,i} + \frac{\Delta_\eta}{6\,i} - 32B_0\left[(2\hat{m}+m_s)\,L_6 + \hat{m}L_8\right]\right\}$$

$$A_K = \frac{\overset{\circ}{M}{}_K^2}{F_0^2}\left\{\frac{\Delta_\pi}{4\,i} + \frac{\Delta_K}{2\,i} - \frac{\Delta_\eta}{12\,i} - 32B_0\left[(2\hat{m}+m_s)\,L_6 + \tfrac{\hat{m}+m_s}{2}L_8\right]\right\} \tag{1.76a}$$

$$A_\eta = \frac{1}{F_0^2}\left\{\overset{\circ}{M}{}_\pi^2\left[\frac{\Delta_\pi}{2\,i} - \frac{\Delta_K}{3\,i} - \frac{\Delta_\eta}{6\,i}\right] + \overset{\circ}{M}{}_\eta^2\,\frac{2\Delta_\eta}{3\,i}\right.$$
$$\left. -32B_0\left[\overset{\circ}{M}{}_\eta^2\left[(2\hat{m}+m_s)\,L_6 + \tfrac{\hat{m}+2m_s}{3}L_8\right] + \frac{4}{9}B_0\,(\hat{m}-m_s)^2\,[3L_7 + L_8]\right]\right\},$$

and

$$B_\pi = \frac{1}{F_0^2}\left\{16B_0\left[(2\hat{m}+m_s)\,L_4 + \hat{m}L_5\right] - \frac{2\Delta_\pi}{3\,i} - \frac{\Delta_K}{3\,i}\right\}$$

$$B_K = \frac{1}{F_0^2}\left\{16B_0\left[(2\hat{m}+m_s)\,L_4 + \tfrac{\hat{m}+m_s}{2}L_5\right] - \frac{\Delta_\pi}{4\,i} - \frac{\Delta_K}{2\,i} - \frac{\Delta_\eta}{4\,i}\right\} \tag{1.76b}$$

$$B_\eta = \frac{1}{F_0^2}\left\{16B_0\left[(2\hat{m}+m_s)\,L_4 + \tfrac{\hat{m}+2m_s}{3}L_5\right] - \frac{\Delta_K}{i}\right\}.$$

The coefficients depend on the coupling constants L_j and on the loop integrals Δ_π, Δ_K, Δ_η. The coupling constants L_j originate from the evaluation of the tree graph while Δ_π, Δ_K, Δ_η from the evaluation of the tadpole diagram. By means of dimensional regularization we can separate the loop integrals in divergent and finite parts,

$$\frac{\Delta_P}{i} = \int \frac{\mathrm{d}^d k}{i\,(2\pi)^d}\,\frac{1}{\overset{\circ}{M}{}_P^2 - k^2} = \frac{\overset{\circ}{M}{}_P^2}{N}\left[2N\,\lambda(\mu) + \overset{\circ}{\ell}_P\right], \qquad \text{for} \quad P = \pi, K, \eta. \tag{1.77}$$

Here, $N = (4\pi)^2$, $\overset{\circ}{\ell}_P = 2\,\log(\overset{\circ}{M}_P/\mu)$ and $\lambda(\mu)$ is given in Eq. (1.58). The divergent part contains $\lambda(\mu)$ and in the calculation of masses, is absorbed by the redefinition (1.59) of the coupling constants L_j. The finite part contains $\overset{\circ}{\ell}_P$ and depends logarithmically on the renormalization scale μ. In the mass calculation, this dependence exactly cancels out with the μ-dependence of the renormalized LEC $L_j^{\mathrm{r}}(\mu)$. Note that the loop integral (1.77) count as the square of a momentum because the finite part is proportional to a mass square. This confirms the Weinberg counting scheme (1.55) which for each loop counts $\mathcal{O}(p^2)$.

Using Eq. (1.72) we now calculate the masses at NLO. We insert the expressions (1.76) and retain terms up to $\mathcal{O}(p^4)$. The divergences are absorbed by the redefinition (1.59) and we obtain

$$
\begin{aligned}
M_\pi^2 &= \overset{\circ}{M}{}_\pi^2 + \frac{\overset{\circ}{M}{}_\pi^2}{NF_0^2}\left\{\frac{\overset{\circ}{\ell}_\pi \overset{\circ}{M}{}_\pi^2}{2} - \frac{\overset{\circ}{\ell}_K \overset{\circ}{M}{}_\eta^2}{6} + 16NB_0\Big[(2\hat{m}+m_s)[2L_6^{\mathrm{r}} - L_4^{\mathrm{r}}] + \hat{m}[2L_8^{\mathrm{r}} - L_5^{\mathrm{r}}]\Big]\right\} \\
M_K^2 &= \overset{\circ}{M}{}_K^2 + \frac{\overset{\circ}{M}{}_K^2}{NF_0^2}\left\{\frac{\overset{\circ}{\ell}_\eta \overset{\circ}{M}{}_\eta^2}{3} + 16NB_0\Big[(2\hat{m}+m_s)[2L_6^{\mathrm{r}} - L_4^{\mathrm{r}}] + \tfrac{\hat{m}+m_s}{2}[2L_8^{\mathrm{r}} - L_5^{\mathrm{r}}]\Big]\right\} \\
M_\eta^2 &= \overset{\circ}{M}{}_\eta^2 - \frac{\overset{\circ}{M}{}_\pi^2}{6NF_0^2}\Big[3\overset{\circ}{\ell}_\pi \overset{\circ}{M}{}_\pi^2 - 2\overset{\circ}{\ell}_K \overset{\circ}{M}{}_K^2 - \overset{\circ}{\ell}_\eta \overset{\circ}{M}{}_\eta^2\Big] + \frac{128}{9}\frac{B_0^2}{F_0^2}(\hat{m}-m_s)^2[3L_7^{\mathrm{r}} + L_8^{\mathrm{r}}] \\
&\quad + \frac{\overset{\circ}{M}{}_\eta^2}{NF_0^2}\left\{\overset{\circ}{\ell}_K \overset{\circ}{M}{}_K^2 - \frac{2\overset{\circ}{\ell}_\eta \overset{\circ}{M}{}_\eta^2}{3} + 16NB_0\Big[(2\hat{m}+m_s)[2L_6^{\mathrm{r}} - L_4^{\mathrm{r}}] + \tfrac{\hat{m}+2m_s}{3}[2L_8^{\mathrm{r}} - L_5^{\mathrm{r}}]\Big]\right\}.
\end{aligned}
\tag{1.78}
$$

These expressions coincide with the results of Ref. [11]. One can easily show that the expressions do not depend on the renormalization scale: the derivative with respect to μ vanishes.

1.4.2 Decay Constants

The decay constant of a pseudoscalar state $|\phi_b\rangle$ is defined by the matrix element,

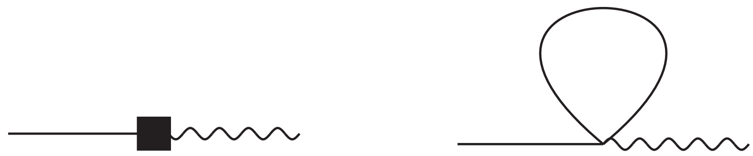
$$\langle 0|\, A_a^\mu(x)\,|\phi_b(p)\rangle = i\, p^\mu\, F_{ab}\, \mathrm{e}^{-ipx}, \tag{1.79}$$

where F_{ab} denotes the decay constant. Without loss of generality we can set $x = 0$ and define

$$\mathscr{A}_{ab}^\mu := \langle 0|\, A_a^\mu(0)\,|\phi_b(p)\rangle = i\, p^\mu\, F_{ab}. \tag{1.80}$$

In ChPT the matrix element $\mathscr{A}_{ab}^\mu$ can be evaluated taking the functional derivatives of the generating functional with respect to a^μ and then, setting $v^\mu = a^\mu = p = 0$, $s = \mathcal{M}$. At leading order, the matrix element gives the same result for all pseudoscalar mesons: the decay constant is $F_{ab} = \delta_{ab}F_0$, see Ref. [11]. This result coincides with the expression in chiral limit, cfr. Eq. (1.32).

At NLO the matrix element $\mathscr{A}_{ab}^\mu$ receives additional contributions from the diagrams of Fig. 1.3. The diagrams are similar to those encountered in the calculation of masses but now one external line represents the axialvector currents. Altogether, they contribute to



(a) Tree graph. *(b) Tadpole diagram.*

Figure 1.3: Contributions to the matrix elements of the axialvector decay at NLO. Solid lines stand for pseudoscalar mesons while wave lines represent the axialvector currents. The square corresponds to a vertex of $\mathcal{L}_4$ whereas the intersection of four lines corresponds to a vertex of $\mathcal{L}_2$.

the matrix elements of pseudoscalar mesons as

$$\begin{aligned}
\mathscr{A}_\pi^\mu &= ip^\mu \frac{1}{F_0}\left\{16B_0\left[(2\hat{m}+m_s)\,L_4+\hat{m}L_5\right]-\frac{2}{3}\left[2\,\frac{\Delta_\pi}{i}+\frac{\Delta_K}{i}\right]\right\}+ip^\mu F_0\,\sqrt{Z_\pi}\\
\mathscr{A}_K^\mu &= ip^\mu \frac{1}{F_0}\left\{16B_0\left[(2\hat{m}+m_s)\,L_4+\tfrac{\hat{m}+m_s}{2}L_5\right]-\left[\frac{\Delta_\pi}{2\,i}+\frac{\Delta_K}{i}+\frac{\Delta_\eta}{2\,i}\right]\right\}+ip^\mu F_0\,\sqrt{Z_K}\\
\mathscr{A}_\eta^\mu &= ip^\mu \frac{1}{F_0}\left\{16B_0\left[(2\hat{m}+m_s)\,L_4+\tfrac{\hat{m}+2m_s}{3}L_5\right]-2\,\frac{\Delta_K}{i}\right\}+ip^\mu F_0\,\sqrt{Z_\eta}.
\end{aligned} \tag{1.81}$$

Here, Z_π, Z_K, Z_η are the renormalization constants of pseudoscalar mesons at NLO and can be calculated from Eq. (1.74) inserting the coefficients (1.76). The coupling constants L_j identify the contribution of the tree graph while loop integrals Δ_π, Δ_K, Δ_η the contribution of the tadpole diagram.

The decay constants can be extracted from Eq. (1.81) contracting the matrix elements with $-ip_\mu$ and dividing by the mass square of the external meson. Retaining terms up to $\mathcal{O}(p^4)$ we obtain,

$$\begin{aligned}
F_\pi &= F_0\left\{1+\frac{1}{NF_0^2}\left[8NB_0\left[(2\hat{m}+m_s)L_4^{\mathrm{r}}+\hat{m}L_5^{\mathrm{r}}\right]-\mathring{\ell}_\pi\mathring{M}_\pi^2-\frac{\mathring{\ell}_K\mathring{M}_K^2}{2}\right]\right\}\\
F_K &= F_0\left\{1+\frac{1}{NF_0^2}\left[8NB_0\left[(2\hat{m}+m_s)L_4^{\mathrm{r}}+\tfrac{\hat{m}+m_s}{2}L_5^{\mathrm{r}}\right]\right]\right.\\
&\qquad\left.-\frac{3}{8NF_0^2}\left[\mathring{\ell}_\pi\mathring{M}_\pi^2+2\mathring{\ell}_K\mathring{M}_K^2+\mathring{\ell}_\eta\mathring{M}_\eta^2\right]\right\}\\
F_\eta &= F_0\left\{1+\frac{1}{NF_0^2}\left[8NB_0\left[(2\hat{m}+m_s)L_4^{\mathrm{r}}+\tfrac{\hat{m}+2m_s}{3}L_5^{\mathrm{r}}\right]-\frac{3\mathring{\ell}_K\mathring{M}_K^2}{2}\right]\right\}.
\end{aligned} \tag{1.82}$$

These expressions coincide with the results of Ref. [11]. Also in this case, one can show that the expressions do not depend on the renormalization scale μ.

1.4.3 Pseudoscalar Coupling Constants

The coupling constant of a pseudoscalar state $|\phi_b\rangle$ is defined by the matrix element,

$$\mathscr{G}_{ab} = \langle 0| P_a(0) |\phi_b(p)\rangle \,. \tag{1.83}$$

In ChPT, this matrix element can be evaluated taking the functional derivative with respect to p and then, setting $v^\mu = a^\mu = p = 0$, $s = \mathcal{M}$. At leading order the matrix element gives the same coupling constant for all pseudoscalar mesons, namely $\mathscr{G}_{ab} = \delta_{ab} G_0$ with $G_0 = 2B_0F_0$, see Ref. [11]. At NLO the coupling constants differ according to the pseudoscalar meson under consideration. One obtains

$$\begin{aligned}
G_\pi = G_0\Bigg\{1 + \frac{1}{NF_0^2}\Big[8NB_0\Big[(2\hat{m}+m_s)[4L_6^{\rm r} - L_4^{\rm r}] + \hat{m}[4L_8^{\rm r} - L_5^{\rm r}]\Big]\Big]& \\
- \frac{1}{2NF_0^2}\Big[\mathring{\ell}_\pi \mathring{M}_\pi^2 + \mathring{\ell}_K \mathring{M}_K^2 + \frac{\mathring{\ell}_\eta \mathring{M}_\eta^2}{3}\Big]\Bigg\}& \\
G_K = G_0\Bigg\{1 + \frac{1}{NF_0^2}\Big[8NB_0\Big[(2\hat{m}+m_s)[4L_6^{\rm r} - L_4^{\rm r}] + \tfrac{\hat{m}+m_s}{2}[4L_8^{\rm r} - L_5^{\rm r}]\Big]\Big]& \\
- \frac{3}{8NF_0^2}\Big[\mathring{\ell}_\pi \mathring{M}_\pi^2 + 2\mathring{\ell}_K \mathring{M}_K^2 + \frac{\mathring{\ell}_\eta \mathring{M}_\eta^2}{9}\Big]\Bigg\}& \\
G_\eta = G_0\Bigg\{1 + \frac{1}{NF_0^2}\Big[8NB_0\Big[(2\hat{m}+m_s)[4L_6^{\rm r} - L_4^{\rm r}] + \tfrac{\hat{m}+2m_s}{3}[4L_8^{\rm r} - L_5^{\rm r}]\Big]\Big]& \\
- \frac{1}{2NF_0^2}\Big[\mathring{\ell}_\pi \mathring{M}_\pi^2 + \frac{\mathring{\ell}_K \mathring{M}_K^2}{3} + \mathring{\ell}_\eta \mathring{M}_\eta^2\Big]\Bigg\}&.
\end{aligned} \tag{1.84}$$

These results were recently presented in Ref. [38]. Here, we show an alternative way to obtain these results relying on chiral Ward identities.

From Ref. [10,11] we know that the matrix elements of the axialvector decay are related to those of the pseudoscalar decay through

$$\begin{aligned}
&\partial_\mu \langle 0| A_a^\mu(0) |\phi_b(p)\rangle = \hat{m}\,\langle 0| P_a(0) |\phi_b(p)\rangle\,, && a,b = 1,2,3 \\
&\partial_\mu \langle 0| A_c^\mu(0) |\phi_d(p)\rangle = \tfrac{\hat{m}+m_s}{2}\,\langle 0| P_c(0) |\phi_d(p)\rangle\,, && c,d = 4,5,6,7 \\
&\partial_\mu \langle 0| A_8^\mu(0) |\phi_8(p)\rangle = \tfrac{\hat{m}+2m_s}{3}\,\langle 0| P_8(0) |\phi_8(p)\rangle + \sqrt{2}\,\tfrac{\hat{m}-m_s}{3}\,\langle 0| P_0(0) |\phi_8(p)\rangle\,.
\end{aligned} \tag{1.85}$$

These identities are a consequence of chiral symmetry and hold to all order in ChPT. The identities for $a, b = 1, 2, 3$ concern pions; those for $c, d = 4, 5, 6, 7$ concern kaons and the last identity concerns the eta meson. On the left-hand side the derivative of the matrix elements is proportional to the product of the mass with the decay constant. On the right-hand side the matrix elements are proportional to the pseudoscalar coupling constants. We bring the pseudoscalar coupling constants on the left-hand side of the identities and isolate the rest on the right-hand side. We find

$$G_\pi = \hat{m}^{-1} M_\pi^2 F_\pi \tag{1.86a}$$

$$G_K = \left[\tfrac{\hat{m}+m_s}{2}\right]^{-1} M_K^2 F_K \tag{1.86b}$$

$$G_\eta = \left[\tfrac{\hat{m}+2m_s}{3}\right]^{-1} \left[M_\eta^2 F_\eta - \sqrt{2}\,\tfrac{\hat{m}-m_s}{3}\, G_{0,\eta}\right]. \tag{1.86c}$$

Apart from $G_{0,\eta}$ we already know all other quantities up to NLO. The matrix element $G_{0,\eta} \mathrel{\widehat{=}} \langle 0 | P_0(0) | \phi_8(p) \rangle$ can be determined applying the functional method. The result is

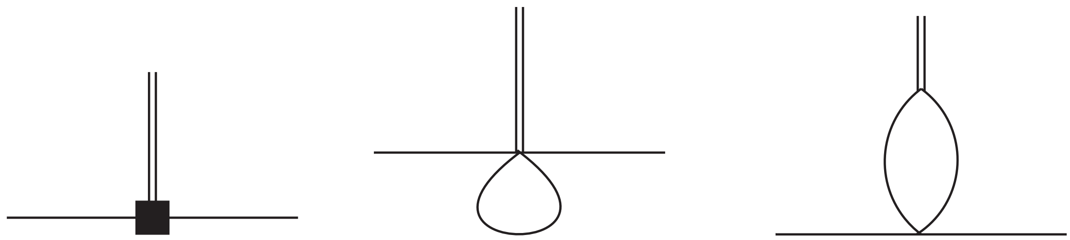
$$G_{0,\eta} = G_0 \frac{\sqrt{2}}{6NF_0^2} \left[64NB_0(\hat{m} - m_s)[3L_7^{\mathrm{r}} + L_8^{\mathrm{r}}] - 3\mathring{\ell}_\pi \mathring{M}_\pi^2 + 6\mathring{\ell}_K \mathring{M}_K^2 + \mathring{\ell}_\eta \mathring{M}_\eta^2\right]. \tag{1.87}$$

Note that $G_{0,\eta}$ has no contribution at leading order but only from NLO onwards. Knowing all quantities of the right-hand side of Eq. (1.86) we determine G_π, G_K, G_η. We insert the expressions (1.78, 1.82, 1.87) and retain terms up to $\mathcal{O}(p^4)$. We obtain the results (1.84).

We may reexpress the results (1.84) in terms of quantities at NLO. We insert the expressions (1.67, 1.78, 1.82) and retain terms up to $\mathcal{O}(p^4)$. We find,

$$\begin{aligned}
G_\pi &= G_0 \Bigg\{ 1 + \frac{1}{NF_\pi^2}\left[4N\Big[(M_\pi^2 + 2M_K^2)[4L_6^{\mathrm{r}} - L_4^{\mathrm{r}}] + M_\pi^2[4L_8^{\mathrm{r}} - L_5^{\mathrm{r}}]\Big]\right] \\
&\qquad - \frac{1}{2NF_\pi^2}\left[\ell_\pi M_\pi^2 + \ell_K M_K^2 + \frac{\ell_\eta M_\eta^2}{3}\right]\Bigg\} \\
G_K &= G_0 \Bigg\{ 1 + \frac{1}{NF_\pi^2}\left[4N\Big[(M_\pi^2 + 2M_K^2)[4L_6^{\mathrm{r}} - L_4^{\mathrm{r}}] + M_K^2[4L_8^{\mathrm{r}} - L_5^{\mathrm{r}}]\Big]\right] \\
&\qquad - \frac{3}{8NF_\pi^2}\left[\ell_\pi M_\pi^2 + 2\ell_K M_K^2 + \frac{\ell_\eta M_\eta^2}{9}\right]\Bigg\} \\
G_\eta &= G_0 \Bigg\{ 1 + \frac{1}{NF_\pi^2}\left[4N\Big[(M_\pi^2 + 2M_K^2)[4L_6^{\mathrm{r}} - L_4^{\mathrm{r}}] + M_\eta^2[4L_8^{\mathrm{r}} - L_5^{\mathrm{r}}]\Big]\right] \\
&\qquad - \frac{1}{2NF_\pi^2}\left[\ell_\pi M_\pi^2 + \frac{\ell_K M_K^2}{3} + \ell_\eta M_\eta^2\right]\Bigg\}.
\end{aligned} \tag{1.88}$$

Here, $\ell_P = 2\log(M_P/\mu)$ with $P = \pi, K, \eta$. We observe that the contributions at NLO appear with a prefactor $1/(NF_\pi^2) = (4\pi F_\pi)^{-2}$. This suggests that the scale of ChPT is $\Lambda_\chi = 4\pi F_\pi \approx 1.2$ GeV, see Ref. [113]. In the remainder we will use that scale and expand physical quantities in powers of $1/\Lambda_\chi$.



(a) Tree graph. *(b) Tadpole diagram.* *(c) Fish diagram.*

Figure 1.4: Contributions to matrix elements of pion form factors at NLO. Single solid lines stand for pions while double solid lines represent the scalar densities (or the vector currents). The square corresponds to a vertex of $\mathcal{L}_4$ whereas the intersection of various lines corresponds to a vertex of $\mathcal{L}_2$.

1.4.4 Pion Form Factors

As a last application we discuss the form factors of pions. In this case we restrict the group to $\mathrm{G}_\chi = \mathrm{SU}(2)_L \times \mathrm{SU}(2)_R \times \mathrm{U}(1)_V$ and consider only $N_\mathrm{f} = 2$ light flavors. The mass and decay constant can be calculated in the same way as before. At NLO we find

$$\begin{aligned} M_\pi^2 &= M^2 \left[1 - \frac{M^2}{2NF^2}\bar{\ell}_3 + \mathcal{O}(M^4)\right] \\ F_\pi &= F\left[1 + \frac{M^2}{NF^2}\bar{\ell}_4 + \mathcal{O}(M^4)\right]. \end{aligned} \tag{1.89}$$

Here, $M^2 = 2B\hat{m}$, $N = (4\pi)^2$ and B, F, $\bar{\ell}_j$ were introduced in Section 1.3.3.

According to Ref. [10] the form factors are defined by the matrix elements

$$\begin{aligned} \langle \pi_b(p')|\, S_0\, |\pi_a(p)\rangle &= \delta_{ab}\, F_S(q^2) \\ \langle \pi_b(p')|\, V_c^\mu\, |\pi_a(p)\rangle &= i\epsilon_{abc}(p' + p)^\mu\, F_V(q^2), \end{aligned} \tag{1.90}$$

where $q^\mu = (p' - p)^\mu$ is the momentum transfer. In ChPT these matrix elements can be evaluted taking the functional derivatives with respect to s (resp. v^μ) and then, setting $v^\mu = a^\mu = p = 0$, $s = \mathcal{M}$. At leading order one obtains,

$$\begin{aligned} F_S(q^2) &= 2B \\ F_V(q^2) &= 1. \end{aligned} \tag{1.91}$$

The form factors are constant and do not depend on the momentum transfer q^μ.

At NLO the matrix elements receive additional contributions from the diagrams of Fig. 1.4. The diagrams have an external double line representing the scalar densitities (resp. the vector currents). They contribute to the pion form factors as

$$\begin{aligned} F_S(q^2) &= F_S(0)\left\{1 + \frac{M_\pi^2}{NF_\pi^2}\left[N\left(\frac{q^2}{M_\pi^2} - \frac{1}{2}\right)\bar{J}(q^2) + \frac{q^2}{M_\pi^2}\left(\bar{\ell}_4 - 1\right)\right]\right\} + \mathcal{O}(q^4) \\ F_V(q^2) &= 1 + \frac{M_\pi^2}{6NF_\pi^2}\left[N\left(\frac{q^2}{M_\pi^2} - 4\right)\bar{J}(q^2) + \frac{q^2}{M_\pi^2}\left(\bar{\ell}_6 - \frac{1}{3}\right)\right] + \mathcal{O}(q^4), \end{aligned} \tag{1.92}$$

where

$$F_S(0) = 2B\left[1 - \frac{M_\pi^2}{NF_\pi^2}\left(\bar{\ell}_3 - \frac{1}{2}\right)\right] + \mathcal{O}(M_\pi^4). \tag{1.93}$$

These expressions coincide with the results of Ref. [10]. The function $\bar{J}(q^2)$ is the finite part of the loop integral defined in Eq. (D.19). The form factors depend on the square of the momentum transfer and are invariant under rotations of q^μ. In position space this rotation invariance implies that the charge distribution depends on the radial direction but not on the angular ones. At $q^2 = 0$ the charge distribution becomes pointlike and the form factors satisfy

$$F_S(0) = \frac{\partial M_\pi^2}{\partial \hat{m}} \tag{1.94a}$$

$$F_V(0) = 1. \tag{1.94b}$$

The first relation follows from the Feynman–Hellman Theorem [39,40] while the second one is a consequence of the (electromagnetic) gauge symmetry and Lorentz invariance [114]. For $q^2 \ll 4M_\pi^2$ we can expand the form factors in power series of q^2:

$$F_X(q^2) = F_X(0)\left[1 + \frac{q^2}{6}\langle r^2\rangle_X^\pi + q^4 c_X^\pi + \mathcal{O}(q^6)\right], \tag{1.95}$$

where $X = S, V$. The linear coefficient $\langle r^2\rangle_X^\pi$ is the square radius and can be determined from the derivative of the form factor with respect to q^2. The quadratic coefficient c_X^π is the curvature of the form factor and can be determined from the double derivative. These quantities are known at two loops [115] and at the lowest order, their expressions are

$$\begin{aligned} \langle r^2\rangle_S^\pi &= \frac{M_\pi^2}{NF_\pi^2}\left(6\,\bar{\ell}_4 - \frac{13}{2}\right) \qquad & c_S^\pi &= \frac{19}{120}\frac{M_\pi^2}{NF_\pi^2} \\ \langle r^2\rangle_V^\pi &= \frac{M_\pi^2}{NF_\pi^2}(\bar{\ell}_6 - 1) \qquad & c_V^\pi &= \frac{1}{60}\frac{M_\pi^2}{NF_\pi^2}. \end{aligned} \tag{1.96}$$

Chapter 2

ChPT in Finite Volume

2.1 Overview of Finite Volume Effects

Numerical simulations of Lattice QCD are performed in a volume of finite extent. The volume is usually a finite cubic box on which boundary conditions are imposed. The choice of boundary conditions depends on the properties of the system and in particular, on the symmetry of the action $\mathcal{S}$. Mostly employed are periodic boundary conditions (PBC) which require periodic fields within the cubic box,

$$q(x + L\hat{e}_j) = q(x), \qquad j = 1, 2, 3. \tag{2.1}$$

Here, L is the side length of the cubic box and $\hat{e}^{\mu}_j = \delta^{\mu}{}_j$ are unit spatial vectors of position space. Requiring periodic fields ensures that the action is single valued within the box and that physical observables can be evaluated unambiguously.

In momentum space the periodicity of the fields corresponds to a discretization of the momenta. The spatial components of the momenta become discrete and take values

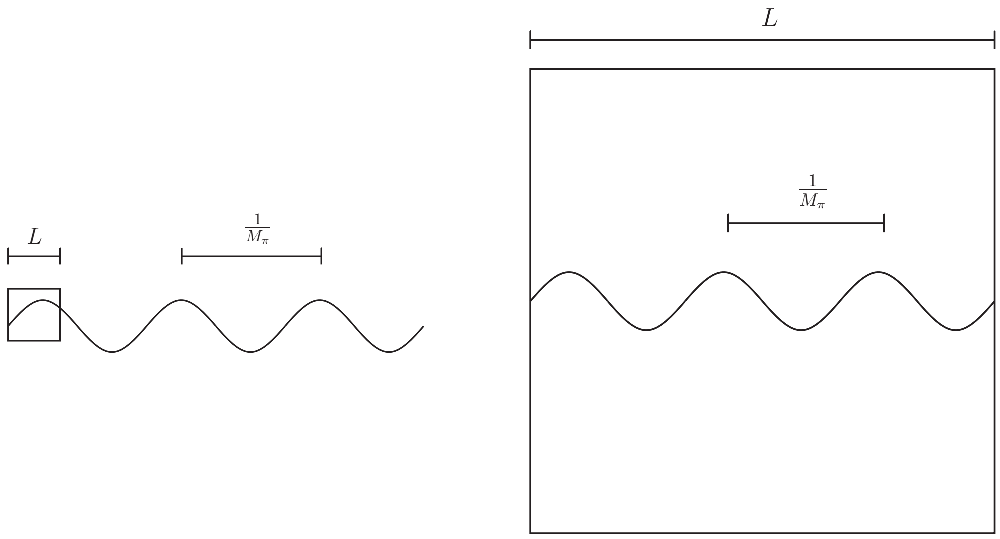
$$\vec{p} = \frac{2\pi}{L}\vec{m}, \qquad \vec{m} \in \mathbb{Z}^3. \tag{2.2}$$

As spatial components are discrete one can not arbitrarily boost or rotate a momentum. Lorentz invariance is broken. However, there is a subgroup of Lorentz transformations which still survives and remains intact: the subgroup of cubic rotations (i.e. spatial rotations of 90°). This subgroup leaves the system invariant and generates the so-called cubic invariance.

The momentum discretization introduces a new scale: $1/L$. If we want to apply ChPT we must consider momenta smaller than the characteristic scale, i.e. $|\vec{p}| \ll \Lambda_\chi$. Taking $\Lambda_\chi = 4\pi F_\pi$, one obtains the following quantitative condition,

$$\frac{2\pi}{L} \ll 4\pi F_\pi \quad \Longrightarrow \quad L \gg \frac{1}{2F_\pi} \approx 1 \text{ fm}, \tag{2.3}$$

where on left-hand side, one has inserted Eq. (2.2) in the first non-zero mode $|\vec{m}| = 1$, see Ref. [116]. This condition guarantees that ChPT is applicable in finite volume. However, it gives no information on how much L must be larger than 1 fm.



(a) ϵ-regime. *(b) p-regime.*

Figure 2.1: Propagation of pions in finite volume. In the ϵ-regime (a) the Compton wavelength of pions is larger than the side length L and pions can not properly propagates within the volume. In the p-regime (b) the Compton wavelength is smaller than L and pions propagate within the volume in a periodic way.

In Ref. [19–21] Gasser and Leutwyler showed how to apply ChPT in finite volume. They proved that for a large enough volume the effective chiral Lagrangian and the values of LEC remain the same as in infinite volume. This, despite the breaking of Lorentz invariance. A symmetry argument demonstrates that all breaking terms disappear and the effective Lagrangian is the same as in infinite volume. The only changes concern the counting scheme and the propagators. The counting scheme now accommodates the new scale $1/L$ and the propagators are modified by discrete momenta. To introduce such changes there are two possible regimes defined by the size of the product $M_\pi L$:

$$\begin{aligned} M_\pi L &\ll 1 \qquad \epsilon\text{-regime} \\ M_\pi L &\gg 1 \qquad p\text{-regime.} \end{aligned} \tag{2.4}$$

In the ϵ-regime, M_π is less than $1/L$. The mass is a small quantity compared with spatial momenta, see Eq. (2.2). The counting scheme is completely modified so that it accommodates the mass resp. the side length as $M_\pi \sim \mathcal{O}(\epsilon^2)$ resp. $1/L \sim \mathcal{O}(\epsilon)$, see Ref. [20]. The situation is qualitatively sketched in Fig. 2.1a. The (reduced) Compton wavelength $1/M_\pi$ of pions[1] is larger than L. Pions encounter the boundaries of the box before they can properly propagate and feel the presence of the volume strongly. The propagation is completely deformed and propagators look very different from those in

[1]Here, "pions" generically refers to the Goldstone bosons arising from the spontaneous breaking of the chiral symmetry.

infinite volume. As we will work on the other regime (i.e. $M_\pi L \gg 1$) we refer the reader to [20, 117–119] for more information about the ϵ-regime.

In the p-regime, M_π is larger than $1/L$. Here, the counting scheme of infinite volume can be applied with the additional rule $1/L \sim \mathcal{O}(p)$, see Ref. [21]. Now, the Compton wavelength $1/M_\pi$ is smaller than L and pions[2] can propagate within the box. There is a non-zero probability that they reach the boundaries and wind around the volume, as sketched in Fig. 2.1b. The propagation is then periodic. The expressions of propagators are similar as those in infinite volume and the only modification is that integrals over spatial components are replaced by sums over discrete values,

$$\Delta_{\pi,L}(x) = \frac{1}{L^3} \sum_{\substack{\vec{k}=\frac{2\pi}{L}\vec{m} \\ \vec{m}\in\mathbb{Z}^3}} \int_{\mathbb{R}} \frac{\mathrm{d}k_0}{(2\pi)} \frac{\mathrm{e}^{-ikx}}{M_\pi^2 - k^2 - i\epsilon}. \tag{2.5}$$

By means of the Poisson resummation formula [117]:

$$\frac{1}{L^3} \sum_{\substack{\vec{k}=\frac{2\pi}{L}\vec{m} \\ \vec{m}\in\mathbb{Z}^3}} g(\vec{k}\,) = \sum_{\vec{n}\in\mathbb{Z}^3} \int_{\mathbb{R}^3} \frac{\mathrm{d}^3k}{(2\pi)^3} g(\vec{k}\,)\, \mathrm{e}^{iL\vec{n}\vec{k}}, \tag{2.6}$$

one can reexpress the propagator as

$$\begin{aligned} \Delta_{\pi,L}(x) &= \sum_{\vec{n}\in\mathbb{Z}^3} \int_{\mathbb{R}^3} \frac{\mathrm{d}^4k}{(2\pi)^4} \frac{\mathrm{e}^{-ikx}}{M_\pi^2 - k^2 - i\epsilon}\, \mathrm{e}^{iL\vec{n}\vec{k}} \\ &= \sum_{\vec{n}\in\mathbb{Z}^3} \Delta_\pi(x + nL), \end{aligned} \tag{2.7}$$

where in the argument $n^\mu = \binom{0}{\vec{n}}$ is a Lorentz vector of integer numbers and $\Delta_\pi(x)$ is the propagator in infinite volume. There is a nice interpretation of the numbers $\vec{n} \in \mathbb{Z}^3$: each component n^j with $j = 1, 2, 3$ gives the number of times the pion winds around the volume in the direction x^j. For instance, pions winding around the volume once are associated to the number $|\vec{n}| = 1$. Pions not winding around the volume are associated to $|\vec{n}| = 0$ and they contribute as in infinite volume. Note that the expressions (2.5, 2.7) are both periodic and satisfy: $\Delta_{\pi,L}(x + L\hat{e}_j) = \Delta_{\pi,L}(x)$ for $j = 1, 2, 3$.

Although the propagators are periodic, physical observables can be calculated in a similar way as in infinite volume. Tree graphs produce exactly the same contributions. On the contrary, loop diagrams generate additional contributions which shift the results of physical observables in finite volume. These additional contributions are known as finite volume corrections and are due to the periodicity of propagators. In the p-regime, they depend exponentially on L. As example, the results of the mass resp. decay constant of

[2]See footnote 1 on the page 38.

pions are shifted at NLO from Eqs. (1.78, 1.82) to

$$M_\pi^2(L) = M_\pi^2 \left[1 + \frac{\xi_\pi}{2}\, \mathrm{g}_1(\lambda_\pi) - \frac{\xi_\eta}{6}\, \mathrm{g}_1(\lambda_\eta)\right] \tag{2.8a}$$

$$F_\pi(L) = F_\pi \left[1 - \xi_\pi\, \mathrm{g}_1(\lambda_\pi) - \frac{\xi_K}{2}\, \mathrm{g}_1(\lambda_K)\right], \tag{2.8b}$$

see Ref. [32]. The corrections are here expressed in terms of

$$\mathrm{g}_1(\lambda_P) = \sum_{\substack{\vec{n}\in\mathbb{Z}^3 \\ |\vec{n}|\neq 0}} \frac{4\, K_1(\lambda_P|\vec{n}|)}{\lambda_P|\vec{n}|}, \tag{2.9}$$

where for $P = \pi, K, \eta$ we have defined the parameters $\lambda_P = M_P L$ and $\xi_P = M_P^2/(4\pi F_\pi)^2$. The function $\mathrm{g}_1(\lambda_P)$ depends on the modified Bessel function of the second kind, $K_1(\lambda_P|\vec{n}|)$. As $K_1(x) \sim \sqrt{\pi/x}\, \mathrm{e}^{-x}$ for $x \gg 1$, the corrections decay exponentially in $\lambda_P = M_P L$. We observe that if we keep L fixed, the exponential decay goes faster if M_P increases. Heavy particles do not very contribute to finite volume corrections. The dominant contribution is given by the lightest particle of the spectrum. As expected, the corrections disappear in the limit $L \to \infty$ and one recovers the original results in infinite volume.

2.2 Twisted Boundary Conditions

A strong limitation of PBC is the momentum discretization. Momenta occur only in integer multiples of $2\pi/L$ and are not continuous. This is an hindrance whenever a continuous limit in momenta is needed to extract physical observables. A possible remedy is provided by twisted boundary conditions (TBC), see Ref. [33–36].

We consider 3-light-flavor QCD in a finite cubic box and impose twisted boundary conditions,

$$q_T(x + L\hat{e}_j) = \mathcal{U}_j q_T(x) \qquad \text{where} \quad \hat{e}_j^\mu = \delta^\mu{}_j \quad \text{and} \quad j = 1, 2, 3. \tag{2.10}$$

The subscript T specifies that the quark fields satisfy TBC. The transformations $\mathcal{U}_j$ constitute a symmetry of the action $\mathcal{S}_{\mathrm{QCD}} = \int \mathrm{d}^4x\, \mathcal{L}_{\mathrm{QCD}}$. They leave the Lagrangian $\mathcal{L}_{\mathrm{QCD}}$ invariant and commute with the mass matrix $\mathcal{M} = \mathrm{diag}(m_u, m_d, m_s)$. The precise form of $\mathcal{U}_j$ depends on $\mathcal{M}$ and especially, on the degeneracy of the quark fields. In general, we may consider

$$\mathcal{U}_j = \mathrm{e}^{-iL\hat{e}_j v_\vartheta} \in \mathrm{SU}(3)_V \tag{2.11}$$

with

$$v_\vartheta^\mu = \vartheta_{\bar{a}}^\mu \frac{\lambda_{\bar{a}}}{2}. \tag{2.12}$$

The matrices $\lambda_{\bar{a}}$ represent the generators of $\mathrm{SU}(3)_V$ commuting with $\mathcal{M}$. In the case of three different quark masses, $\lambda_{\bar{a}}$ are the diagonal Gell-Mann matrices, i.e. λ_3, λ_8. Other choices are possible depending on the specific form of the mass matrix[3]. The Lorentz vectors

$$\vartheta^\mu_{\bar{a}} = \begin{pmatrix} 0 \\ \vec{\vartheta}_{\bar{a}} \end{pmatrix}, \qquad \bar{a} = 3, 8, \tag{2.13}$$

are called twisting angles and their spatial components $\vec{\vartheta}_{\bar{a}}$ can be arbitrarily chosen.

For convenience, we redefine the quark fields through

$$q_T(x) = \mathcal{V}(x) q(x), \qquad \text{with} \quad \mathcal{V}(x) = \mathrm{e}^{-i v_\vartheta x}. \tag{2.14}$$

From the condition (2.10) follows that the fields $q(x)$ are periodic and therefore, satisfy $q(x + L\hat{e}_j) = q(x)$ for $j = 1, 2, 3$. The redefinition introduces the twist in the QCD Lagrangian in an explicit way,

$$\begin{aligned} \mathcal{L}_{\mathrm{QCD}} &= \bar{q}_T(x) \left[i\not{D} - \mathcal{M} \right] q_T(x) - \frac{1}{4} G_{\mu\nu,a} G^{\mu\nu}_a \\ &= \bar{q}(x) \left[i\mathcal{V}^\dagger(x) \not{D} \mathcal{V}(x) - \mathcal{M} \right] q(x) - \frac{1}{4} G_{\mu\nu,a} G^{\mu\nu}_a \\ &= \bar{q}(x) \big[i \underbrace{\left(\not{D} - i\not{v}_\vartheta \right)}_{=:\hat{\not{D}}} - \mathcal{M} \big] q(x) - \frac{1}{4} G_{\mu\nu,a} G^{\mu\nu}_a . \end{aligned} \tag{2.15}$$

The twist enters as a constant vector field v^μ_ϑ and couples to the periodic fields $q(x)$. We can either impose the condition (2.10) and work with $\mathcal{L}_{\mathrm{QCD}}$ in its original form or redefine the fields as periodic ones and introduce v^μ_ϑ in the Lagrangian. Both approaches are equivalent.

The effect of the twist can be inferred from the new Dirac operator containing $\hat{\not{D}}$. The momenta of quark fields are shifted by the twisting angles according to their flavor. For the three light flavors we have

$$\begin{aligned} \vartheta^\mu_u &= \frac{\vartheta^\mu_3}{2} + \frac{\vartheta^\mu_8}{2\sqrt{3}} \\ \vartheta^\mu_d &= -\frac{\vartheta^\mu_3}{2} + \frac{\vartheta^\mu_8}{2\sqrt{3}} \\ \vartheta^\mu_s &= -\frac{\vartheta^\mu_8}{\sqrt{3}} . \end{aligned} \tag{2.16}$$

The twisting angles ϑ^μ_u, ϑ^μ_d, ϑ^μ_s vary continuously as the spatial components $\vec{\vartheta}_{\bar{3}}$, $\vec{\vartheta}_{\bar{8}}$ can be arbitrarily chosen. In this way, the spatial momenta are shifted to continuous values which differ from integer multiples of $2\pi/L$.

Twisted boundary conditions introduce twisting angles and break various symmetries. The cubic invariance in momentum space is broken. More generally, all symmetries not commuting with v^μ_ϑ are broken. For three different quark masses, these are: the vector symmetry $\mathrm{SU}(3)_V$ and the isospin symmetry. Note that in this case, the third isospin

[3] In the isospin limit, we may choose $\lambda_{\bar{a}} = \lambda_1, \lambda_2, \lambda_3, \lambda_8$ since are all commuting with $\mathcal{M}$. Still, this choice breaks the conservation of the electric charge and is not considered in this work.

component I_3, the strangeness S and the electric charge Q_e are still conserved quantities. In addition, there is a new one: as the transformations $\mathcal{U}_j$ constitute a symmetry of the action, at each vertex the sum of incoming and outgoing twisting angles is conserved and amounts to zero, see Ref. [36].

In the effective theory the condition (2.10) implies that the unitary matrix with the fields of pseudoscalar mesons satisfies

$$U_T(x+L\hat{e}_j) = \mathcal{U}_j U_T(x) \mathcal{U}_j^\dagger, \quad j=1,2,3. \tag{2.17}$$

On the right-hand side, the repetition of j does not imply any sum. The subscript T specifies again that the fields satisfy TBC. We redefine the unitary matrix so that the fields are periodic

$$U(x) = \mathcal{V}^\dagger(x) U_T(x) \mathcal{V}(x), \qquad \mathcal{V}(x) = \mathrm{e}^{-iv_\vartheta x}. \tag{2.18}$$

The redefinition introduces the twist in the effective Lagrangian as a constant vector field v_ϑ^μ. Each derivative must be replaced by $\partial^\mu . \mapsto \partial^\mu . - i\left[v_\vartheta^\mu , \, . \,\right]$. At leading order we have

$$\mathcal{L}_2 = \frac{F_0^2}{4} \langle \hat{D}_\mu U (\hat{D}^\mu U)^\dagger + \chi U^\dagger + U\chi^\dagger \rangle \,, \tag{2.19}$$

where

$$\hat{D}^\mu U = D^\mu U - i\left[v_\vartheta^\mu, U\right]. \tag{2.20}$$

The operator $\hat{D}^\mu$ consists of the covariant derivative (1.50) minus the commutator containing the constant vector field v_ϑ^μ. We stress that all fields in (2.19, 2.20) are periodic. The commutator acts on the fields of pseudoscalar mesons in different ways. Pseudoscalar mesons sitting in the diagonal of U commute with v_ϑ^μ and their momenta are untouched by the twist. Pseudoscalar mesons off the diagonal do not commute with v_ϑ^μ and their momenta are shifted by twisting angles,

$$\left[v_\vartheta^\mu, U\right] = \frac{1}{F_0}\begin{pmatrix} 0 & \sqrt{2}\,\vartheta^\mu_{\pi^+}\pi^+ & \sqrt{2}\,\vartheta^\mu_{K^+}K^+ \\ \sqrt{2}\,\vartheta^\mu_{\pi^-}\pi^- & 0 & \sqrt{2}\,\vartheta^\mu_{K^0}K^0 \\ \sqrt{2}\,\vartheta^\mu_{K^-}K^- & \sqrt{2}\,\vartheta^\mu_{\bar{K}^0}\bar{K}^0 & 0 \end{pmatrix} + \mathcal{O}(\Phi^2), \tag{2.21}$$

where

$$\begin{aligned}
\vartheta^\mu_{\pi^+} &= \vartheta^\mu_u - \vartheta^\mu_d = \vartheta^\mu_3 & \vartheta^\mu_{\pi^-} &= -\vartheta^\mu_{\pi^+} \\
\vartheta^\mu_{K^+} &= \vartheta^\mu_u - \vartheta^\mu_s = \frac{\vartheta^\mu_3}{2} + \frac{\sqrt{3}}{2}\vartheta^\mu_8 & \vartheta^\mu_{K^-} &= -\vartheta^\mu_{K^+} \\
\vartheta^\mu_{K^0} &= \vartheta^\mu_d - \vartheta^\mu_s = -\frac{\vartheta^\mu_3}{2} + \frac{\sqrt{3}}{2}\vartheta^\mu_8 & \vartheta^\mu_{\bar{K}^0} &= -\vartheta^\mu_{K^0}.
\end{aligned} \tag{2.22}$$

Momenta of charged pions and kaons are shifted by twisting angles and their spatial components may take continuous values. Note that twisting angles reflect the flavor content of the particles. A pseudoscalar meson with the flavor content $q_f\bar{q}_{f'}$ has the twisting angle $\vartheta^\mu_{q_f\bar{q}_{f'}} = (\vartheta_{q_f} - \vartheta_{q_{f'}})^\mu$. Antiparticles have twisting angles of opposite sign.

Twisting angles enter the expressions of external states and internal propagators [36]. As an example we consider charged pions (kaons have similar expressions). The field redefinition (2.18) implies that the propagators read

$$\Delta_{\pi^\pm,L}(x) = \frac{1}{L^3} \sum_{\substack{\vec{k}=\frac{2\pi}{L}\vec{m} \\ \vec{m}\in\mathbb{Z}^3}} \int_{\mathbb{R}} \frac{\mathrm{d}k_0}{(2\pi)} \frac{\mathrm{e}^{-ikx}}{M_\pi^2 - (k+\vartheta_{\pi^\pm})^2 - i\epsilon}. \tag{2.23}$$

The twisting angles enter the denominator but not the exponential function $\exp(-ikx)$ of the numerator. The propagators are periodic [viz. $\Delta_{\pi^\pm,L}(x+L\hat{e}_j) = \Delta_{\pi^\pm,L}(x)$ for $j=1,2,3$] and obey Klein–Gordon equations[4] with new d'Alembert operators $\hat{\Box}$:

$$\big[\underbrace{(\partial - i\vartheta_{\pi^\pm})^2}_{=:\hat{\Box}} + M_\pi^2\big]\Delta_{\pi^\pm,L}(x) = \delta^{(4)}(x). \tag{2.24}$$

From Eq. (2.23) we see that twisting angles shift the poles in the denominator of propagators. At tree level the poles are shifted to

$$(k+\vartheta_{\pi^\pm})^2 = M_\pi^2. \tag{2.25}$$

Here, M_π^2 is given by Eq. (1.78) and contains the contribution in infinite volume at NLO. We note that in Eq. (2.23) the substitution $k_0 \mapsto -k_0$ and $\vec{k} \mapsto -\vec{k}$ reverse the propagation direction and the sign of the twisting angles. Since antiparticles have twisting angles of opposite sign, we conclude that the propagation of a positive pion with $\vartheta^\mu_{\pi^+}$ in the forward direction of space-time is equivalent to a propagation of a negative pion with $\vartheta^\mu_{\pi^-}$ in the backward direction.

As a concluding remark we observe that PBC are a particular case of TBC. If we set $\vartheta^\mu_{\bar{a}} = 0$ the condition (2.10) reduces to the condition (2.1). This means that we may partly check calculations by taking the limit $\vartheta^\mu_{\bar{a}} \to 0$ and comparing the results with those obtained in finite volume with PBC.

2.3 Finite Volume Corrections with TBC

We consider pseudoscalar mesons in a cubic box with TBC and calculate finite volume corrections with ChPT in the p-regime. The corrections of masses, decay constants, pseudoscalar coupling constants and pion form factors are calculated at NLO. The corrections of masses and decay constants for pions and kaons were first presented in Ref. [36]. Here, we detail the derivations and add results for the eta meson. We compare our expressions with the results of Ref. [38] and explain how they are related with each other. Relying

[4]Without the redefinition (2.18) propagators read as in Eq. (2.23) but twisting angles enter the exponential function of the numerator, as well [e.g. $\mathrm{e}^{-i(k+\vartheta_{\pi^\pm})x}$ for charged pions]. In that case, the propagators satisfy TBC [i.e. $\Delta_{\pi^\pm,L}(x+L\hat{e}_j) = \mathrm{e}^{-iL\hat{e}_j\vartheta_{\pi^\pm}}\Delta_{\pi^\pm,L}(x)$ for $j=1,2,3$] and obey Klein–Gordon equations with the usual d'Alembert operators $\Box := \partial_\mu\partial^\mu$.

on chiral Ward identities, we then calculate the corrections of the pseudoscalar coupling contants. Our expressions coincide with the results obtained from the direct calculation of Ref. [38]. At last, we calculate the corrections of matrix elements of the pion form factors. We show that here, the Feynman–Hellman Theorem [39,40] as well as the Ward–Takahashi identity [41–43] hold in finite volume with TBC. We conclude comparing our expressions with the results of Ref. [37, 38, 52, 120–124].

2.3.1 Masses

To determine the mass corrections at NLO we must evaluate the tadpole diagram of Fig. 1.2b in finite volume. The finite volume discretizes the momenta and introduces twisting angles. The propagators are modified in the measure that integrals over spatial components are replaced by discrete sums and twisting angles enter the denominator. For example, the propagator of the neutral pion has the form of Eq. (2.5) whereas those of charged pions have the form of Eq. (2.23). The discrete sums can be evaluated by means of the Poisson resummation formula (2.6). The different twisting angles force us to distinguish the various particles propagating in the loop of the tadpole diagram as they have propagators of different forms. This elongates a bit the evaluation of the diagram which nonetheless remains straightforward. For convenience, we detail just the derivation of pions; mass corrections of other pseudoscalar mesons can be derived in an analogous way.

In finite volume the tadpole diagram of Fig. 1.2b generates the corrections of the self energies at NLO. For pions, we find

$$\Delta\Sigma_{\pi^0} = \Delta A_{\pi^0} + \Delta B_{\pi^0}\, p^2 + \mathcal{O}(p^6/F_\pi^4) \tag{2.26a}$$

$$\Delta\Sigma_{\pi^\pm} = \Delta A_{\pi^\pm} + \Delta B_{\pi^\pm}\, (p+\vartheta_{\pi^\pm})^2 + 2\,(p+\vartheta_{\pi^\pm})_\mu \Delta\vartheta^\mu_{\pi^\pm} + \mathcal{O}(p^6/F_\pi^4), \tag{2.26b}$$

where we normalize $\Delta\Sigma_{\pi^0}$, $\Delta\Sigma_{\pi^\pm}$ so that they just contain the corrections due to finite volume. The contribution in infinite volume can be found in Eqs. (1.75, 1.76). The coefficients entering the self energies read

$$\begin{aligned}\Delta A_{\pi^0} = {}& \frac{M_\pi^2}{6}\,\xi_\pi\,[3\ \mathrm{g}_1(\lambda_\pi) - 2\ \mathrm{g}_1(\lambda_\pi,\vartheta_{\pi^+})] \\ & + \frac{M_\pi^2}{6}\,\{\xi_K\,[\mathrm{g}_1(\lambda_K,\vartheta_{K^+}) + \mathrm{g}_1(\lambda_K,\vartheta_{K^0})] + \xi_\eta\,\mathrm{g}_1(\lambda_\eta)\}\end{aligned} \tag{2.27a}$$

$$\Delta B_{\pi^0} = -\frac{1}{6}\,\{4\,\xi_\pi\,\mathrm{g}_1(\lambda_\pi,\vartheta_{\pi^+}) + \xi_K\,[\mathrm{g}_1(\lambda_K,\vartheta_{K^+}) + \mathrm{g}_1(\lambda_K,\vartheta_{K^0})]\}\,, \tag{2.27b}$$

and

$$\begin{aligned}\Delta A_{\pi^\pm} = {}& \frac{M_\pi^2}{6}\,\xi_\pi\,[2\ \mathrm{g}_1(\lambda_\pi,\vartheta_{\pi^+}) - \mathrm{g}_1(\lambda_\pi)] \\ & + \frac{M_\pi^2}{6}\,\{\xi_K\,[\mathrm{g}_1(\lambda_K,\vartheta_{K^+}) + \mathrm{g}_1(\lambda_K,\vartheta_{K^0})] + \xi_\eta\,\mathrm{g}_1(\lambda_\eta)\}\end{aligned} \tag{2.28a}$$

$$\Delta B_{\pi^\pm} = -\frac{1}{6}\,\{2\,\xi_\pi\,[\mathrm{g}_1(\lambda_\pi,\vartheta_{\pi^+}) + \mathrm{g}_1(\lambda_\pi)] + \xi_K\,[\mathrm{g}_1(\lambda_K,\vartheta_{K^+}) + \mathrm{g}_1(\lambda_K,\vartheta_{K^0})]\}\,. \tag{2.28b}$$

Here, $\mathrm{g}_1(\lambda_P)$ is the function of Eq. (2.9) and λ_P, ξ_P (with $P = \pi, K, \eta$) are the parameters defined after Eq. (2.9). The function $\mathrm{g}_1(\lambda_P, \vartheta)$ is defined by the difference of the sum in finite volume minus the integral in infinite volume,

$$\frac{1}{L^3} \sum_{\substack{\vec{k}=\frac{2\pi}{L}\vec{m} \\ \vec{m}\in\mathbb{Z}^3}} \int_{\mathbb{R}} \frac{\mathrm{d}k_0}{2\pi} \frac{1}{i\,[M_P^2 - (k+\vartheta)^2]} - \int_{\mathbb{R}^4} \frac{\mathrm{d}^4 k}{(2\pi)^4} \frac{1}{i\,[M_P^2 - (k+\vartheta)^2]} = \frac{M_P^2}{(4\pi)^2}\, \mathrm{g}_1(\lambda_P, \vartheta). \tag{2.29}$$

It can be evaluated by means of the Poisson resummation formula (2.6) and values

$$\mathrm{g}_1(\lambda_P, \vartheta) = \sum_{\substack{\vec{n}\in\mathbb{Z}^3 \\ |\vec{n}|\neq 0}} \frac{4\,K_1(\lambda_P|\vec{n}|)}{\lambda_P|\vec{n}|}\, \mathrm{e}^{iL\vec{n}\vec{\vartheta}}. \tag{2.30}$$

Note that $\mathrm{g}_1(\lambda_P, \vartheta)$ is even in the second argument and thus antiparticles contribute as particles, e.g. $\mathrm{g}_1(\lambda_\pi, \vartheta_{\pi^-}) = \mathrm{g}_1(\lambda_\pi, \vartheta_{\pi^+})$. For vanishing angles, $\mathrm{g}_1(\lambda_P, 0) = \mathrm{g}_1(\lambda_P)$ and we recover the function of Eq. (2.9).

In addition, the self energies of charged pions exhibit extra terms proportional to $\Delta\vartheta^\mu_{\pi^\pm}$. Such terms are not present in finite volume with PBC and feature

$$\Delta\vartheta^\mu_{\pi^\pm} = \pm \left\{ \xi_\pi\, \mathrm{f}_1^\mu(\lambda_\pi, \vartheta_{\pi^+}) + \frac{\xi_K}{2}\, [\mathrm{f}_1^\mu(\lambda_K, \vartheta_{K^+}) - \mathrm{f}_1^\mu(\lambda_K, \vartheta_{K^0})] \right\}. \tag{2.31}$$

The function $\mathrm{f}_1^\mu(\lambda_P, \vartheta)$ is defined by

$$\frac{1}{L^3} \sum_{\substack{\vec{k}=\frac{2\pi}{L}\vec{m} \\ \vec{m}\in\mathbb{Z}^3}} \int_{\mathbb{R}} \frac{\mathrm{d}k_0}{(2\pi)} \frac{(k+\vartheta)^\mu}{i\,[M_P^2 - (k+\vartheta)^2]} = -\frac{M_P^2}{(4\pi)^2}\, \mathrm{f}_1^\mu(\lambda_P, \vartheta), \tag{2.32}$$

and can be evaluated by means of the Poisson resummation formula (2.6):

$$\mathrm{f}_1^\mu(\lambda_P, \vartheta) = \sum_{\substack{\vec{n}\in\mathbb{Z}^3 \\ |\vec{n}|\neq 0}} \frac{4i}{L|\vec{n}|^2}\, n^\mu\, K_2(\lambda_P|\vec{n}|)\, \mathrm{e}^{iL\vec{n}\vec{\vartheta}}, \qquad \text{where} \quad n^\mu = \begin{pmatrix} 0 \\ \vec{n} \end{pmatrix}. \tag{2.33}$$

In Ref. [37] this function[5] was studied in partially quenched ChPT with partially twisted boundary conditions. Despite the different framework we can make similar remarks. The function $\mathrm{f}_1^\mu(\lambda_P, \vartheta)$ decays exponentially in $\lambda_P = M_P L$ and disappears for $L \to \infty$. It is odd in the second argument so that antiparticles contribute with the opposite sign, e.g.

[5]For $j = 1, 2, 3$ the function $\mathrm{f}_1^j(\lambda_P, \vartheta)$ is related to $\mathcal{K}^j_{1/2}(\vartheta, M_P^2)$ of Ref. [37] via

$$\mathrm{f}_1^j(\lambda_P, \vartheta) = -\frac{(4\pi)^2}{2M_P^2}\, \mathcal{K}^j_{1/2}(\vartheta, M_P^2).$$

$\mathrm{f}_1^\mu(\lambda_\pi, \vartheta_{\pi^-}) = -\mathrm{f}_1^\mu(\lambda_\pi, \vartheta_{\pi^+})$. For $\vartheta^\mu = 0$, the summand in Eq. (2.33) becomes odd in $\vec{n}$ and $\mathrm{f}_1^\mu(\lambda_P, \vartheta)$ disappears due to the summation over $\vec{n} \in \mathbb{Z}^3$. This explains why the extra terms $\Delta\vartheta^\mu_{\pi^\pm}$ are not present in finite volume with PBC: they disappear due to the cubic invariance. In general, the function $\mathrm{f}_1^\mu(\lambda_P, \vartheta)$ has non-vanishing components in the directions where ϑ^μ is non-vanishing. In the case that $\vartheta^\mu = \left(\begin{smallmatrix} 0 \\ \vec{\vartheta} \end{smallmatrix}\right)$ with

$$\vec{\vartheta} \in \left\{ \begin{pmatrix} \vartheta \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ \vartheta \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ \vartheta \end{pmatrix}, \frac{1}{\sqrt{2}}\begin{pmatrix} \vartheta \\ \vartheta \\ 0 \end{pmatrix}, \frac{1}{\sqrt{2}}\begin{pmatrix} \vartheta \\ 0 \\ \vartheta \end{pmatrix}, \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ \vartheta \\ \vartheta \end{pmatrix}, \frac{1}{\sqrt{3}}\begin{pmatrix} \vartheta \\ \vartheta \\ \vartheta \end{pmatrix} \right\}, \tag{2.34}$$

$\mathrm{f}_1^\mu(\lambda_P, \vartheta)$ is aligned to ϑ^μ. This fact intimately relates $\mathrm{f}_1^\mu(\lambda_P, \vartheta)$ to ϑ^μ and more in general, the extra terms $\Delta\vartheta^\mu_{\pi^\pm}$ to the twisting angles.

From Eq. (2.26) we observe that the isospin symmetry is broken in the self energies. The twisting angles break the symmetry and lift the degeneracy among pions. In general, $\Delta\Sigma_{\pi^0}$, $\Delta\Sigma_{\pi^+}$, $\Delta\Sigma_{\pi^-}$ have different expressions. At NLO, the breaking affects the coefficients [i.e. $\Delta A_{\pi^0} \neq \Delta A_{\pi^\pm}$ and $\Delta B_{\pi^0} \neq \Delta B_{\pi^\pm}$] as well as the external momenta [i.e. $p^\mu \neq (p + \vartheta_{\pi^\pm})^\mu$ and $(p+\vartheta_{\pi^+})_\mu \Delta\vartheta^\mu_{\pi^+} \neq (p+\vartheta_{\pi^-})_\mu \Delta\vartheta^\mu_{\pi^-}$]. The breaking disappears only for $\vartheta^\mu_{\pi^+} = 0$, namely when the isospin symmetry is restored in the theory as the u-quark and the d-quark have equal twisting angles (i.e. $\vartheta^\mu_u = \vartheta^\mu_d$). Note that in the rest frame (where $\vec{p} = \vec{0}$) the isospin symmetry breaks in a specific way. The first two components are broken but not the third one. Pseudoscalar mesons with $I = |I_3|$ remain degenerate as they are aligned to the third component. For example, charged pions are degenerate and have the same self energies, $\Delta\Sigma_{\pi^+} = \Delta\Sigma_{\pi^-}$. This can be showed setting $p^\mu = \hat{p}^\mu \mathrel{\widehat{=}} \left(\begin{smallmatrix} p^0 \\ \vec{0} \end{smallmatrix}\right)$ in Eq. (2.26b): terms with coefficients $\Delta A_{\pi^\pm}$, $\Delta B_{\pi^\pm}$ become equal due to Eq. (2.28) and terms $2(\hat{p} + \vartheta_{\pi^\pm})_\mu \Delta\vartheta^\mu_{\pi^\pm}$ become equal as well, due to $\vartheta^\mu_{\pi^-} = -\vartheta^\mu_{\pi^+}$, $\Delta\vartheta^\mu_{\pi^-} = -\Delta\vartheta^\mu_{\pi^+}$, see Eqs. (2.22, 2.31).

In finite volume, masses are defined in the usual way. They are given by the poles of the full propagators. In the case of pions, $\Delta\Sigma_{\pi^0}$, $\Delta\Sigma_{\pi^\pm}$ further shift these poles. The pole equation of the neutral pion reads

$$M_\pi^2 - p^2 - \Delta\Sigma_{\pi^0} = 0 \qquad \text{for} \quad p^2 = M^2_{\pi^0}(L), \tag{2.35}$$

where $M_{\pi^0}(L)$ is the mass in finite volume. Inserting (2.26a) in the pole equation we find

$$M^2_{\pi^0}(L) = M_\pi^2 - \Delta A_{\pi^0} - \Delta B_{\pi^0} M_\pi^2 + \mathcal{O}(p^6/F_\pi^4). \tag{2.36}$$

For charged pions, the self energies $\Delta\Sigma_{\pi^\pm}$ exhibit the extra terms $\Delta\vartheta^\mu_{\pi^\pm}$. Currently, there are two distinct treatments for such terms which lead to two different mass definitions, see Ref. [36–38]. In Ref. [36, 37] the extra terms $\Delta\vartheta^\mu_{\pi^\pm}$ were treated as an additive renormalization to the twisting angles and were reabsorbed in the on-shell conditions. This leads to a momentum-independent definition of masses. On the contrary, the authors of Ref. [38] adopt a momentum-dependent definition and treat $\Delta\vartheta^\mu_{\pi^\pm}$ as parts of the mass corrections. At NLO, both definitions are equivalent although they provide different results for the corrections. Here, we adopt the definition of Ref. [36, 37] which is more compact and provides momentum-independent corrections. We start from the pole equations of charged pions,

$$M_\pi^2 - (p + \vartheta_{\pi^\pm})^2 - \Delta\Sigma_{\pi^\pm} = 0, \tag{2.37}$$

and insert (2.26b). Working out the left-hand side we find,

$$
\begin{aligned}
M_\pi^2 - (p+\vartheta_{\pi^\pm})^2 - \Delta\Sigma_{\pi^\pm} &= M_\pi^2 - (p+\vartheta_{\pi^\pm})^2 - 2\,(p+\vartheta_{\pi^\pm})_\mu \Delta\vartheta^\mu_{\pi^\pm} \\
&\qquad - \Delta A_{\pi^\pm} - \Delta B_{\pi^\pm}(p+\vartheta_{\pi^\pm})^2 + \mathcal{O}(p^6/F_\pi^4) \\
&= M_\pi^2 - (p+\vartheta_{\pi^\pm}+\Delta\vartheta_{\pi^\pm})^2 \\
&\qquad - \Delta A_{\pi^\pm} - \Delta B_{\pi^\pm}(p+\vartheta_{\pi^\pm}+\Delta\vartheta_{\pi^\pm})^2 + \mathcal{O}(p^6/F_\pi^4).
\end{aligned}
\tag{2.38}
$$

In the last equality, we have followed Ref. [37] and added terms $\mathcal{O}(p^6/F_\pi^4)$ to complete the momentum squares $(p+\vartheta_{\pi^\pm})^2$ with $\Delta\vartheta^\mu_{\pi^\pm}$. As noted in [37] after completing the momentum squares, the extra terms $\Delta\vartheta^\mu_{\pi^\pm}$ appear as an additive renormalization to the twisting angles $\vartheta^\mu_{\pi^\pm}$. The renormalization terms can be reabsorbed in the on-shell conditions,

$$
p^2_{\pi^\pm}(L) := (p+\vartheta_{\pi^\pm}+\Delta\vartheta_{\pi^\pm})^2 = M^2_{\pi^\pm}(L). \tag{2.39}
$$

Then, the pole equations (2.38) provide the masses in finite volume,

$$
M^2_{\pi^\pm}(L) = M_\pi^2 - \Delta A_{\pi^\pm} - \Delta B_{\pi^\pm} M_\pi^2 + \mathcal{O}(p^6/F_\pi^4). \tag{2.40}
$$

In an analogous way, one can determine the masses of other pseudoscalar mesons in finite volume. For the eta meson one proceeds as for the neutral pion. For kaons one follows the derivation of charged pions and completes the momentum squares as in Eq. (2.38). In that case, the renormalization terms read

$$
\Delta\vartheta^\mu_{K^\pm} = \pm\left\{\frac{\xi_K}{2}\left[2\,\mathrm{f}^\mu_1(\lambda_K,\vartheta_{K^+}) + \mathrm{f}^\mu_1(\lambda_K,\vartheta_{K^0})\right] + \frac{\xi_\pi}{2}\,\mathrm{f}^\mu_1(\lambda_\pi,\vartheta_{\pi^+})\right\} \tag{2.41a}
$$

$$
\left.\begin{matrix}\Delta\vartheta^\mu_{K^0} \\ \Delta\vartheta^\mu_{\bar{K}^0}\end{matrix}\right\} = \pm\left\{\frac{\xi_K}{2}\left[\mathrm{f}^\mu_1(\lambda_K,\vartheta_{K^+}) + 2\,\mathrm{f}^\mu_1(\lambda_K,\vartheta_{K^0})\right] - \frac{\xi_\pi}{2}\,\mathrm{f}^\mu_1(\lambda_\pi,\vartheta_{\pi^+})\right\}. \tag{2.41b}
$$

One can reabsorb these terms in the on-shell conditions and calculate the masses in a similar way as in Eq. (2.40).

We summarize the results and make some concluding remarks on the masses in finite volume. In general, we define the corrections of an observable X as

$$
\delta X = \frac{\Delta X}{X}, \tag{2.42}
$$

where $\Delta X := X(L) - X$ is the difference among the observable evaluated in finite volume and in infinite volume. Accordingly, the mass corrections of pseudoscalar mesons read

$$
\delta M^2_{\pi^0} = \frac{\xi_\pi}{2}\left[2\,\mathrm{g}_1(\lambda_\pi,\vartheta_{\pi^+}) - \mathrm{g}_1(\lambda_\pi)\right] - \frac{\xi_\eta}{6}\,\mathrm{g}_1(\lambda_\eta) \tag{2.43a}
$$

$$
\delta M^2_{\pi^\pm} = \frac{\xi_\pi}{2}\,\mathrm{g}_1(\lambda_\pi) - \frac{\xi_\eta}{6}\,\mathrm{g}_1(\lambda_\eta) \tag{2.43b}
$$

$$
\delta M^2_K = \frac{\xi_\eta}{3}\,\mathrm{g}_1(\lambda_\eta), \tag{2.43c}
$$

and

$$\begin{aligned}\delta M_\eta^2 = \frac{\xi_K}{2}\left[\mathrm{g}_1(\lambda_K, \vartheta_{K^+}) + \mathrm{g}_1(\lambda_K, \vartheta_{K^0})\right] - \frac{2}{3}\,\xi_\eta\,\mathrm{g}_1(\lambda_\eta) \\ + \frac{M_\pi^2}{M_\eta^2}\left\{\frac{\xi_K}{6}\left[\mathrm{g}_1(\lambda_K, \vartheta_{K^+}) + \mathrm{g}_1(\lambda_K, \vartheta_{K^0})\right] + \frac{\xi_\eta}{6}\,\mathrm{g}_1(\lambda_\eta)\right\} \\ - \frac{M_\pi^2}{M_\eta^2}\,\frac{\xi_\pi}{6}\left[\mathrm{g}_1(\lambda_\pi) + 2\,\mathrm{g}_1(\lambda_\pi, \vartheta_{\pi^+})\right].\end{aligned} \tag{2.43d}$$

These expressions are obtained with the mass definition of Ref. [36, 37]. The first three expressions coincide with the results of Ref. [36]. As further check we set $\vartheta^\mu_{\pi^+} = \vartheta^\mu_{K^+} = \vartheta^\mu_{K^0} = 0$ and recover the results[6] for PBC, see Eqs. (94, 95, 96) of Ref. [32]. In Ref. [36] it was pointed out that at this order, the mass corrections decrease exponentially in $\lambda_P = M_P L$ where $P = \pi, K, \eta$. Moreover, the dependence on the twist is a phase factor. The twist can change the sign of overall corrections. This is a consequence of the breaking of the vector symmetry $\mathrm{SU}(3)_V$ due to twisting angles. For instance, $\delta M^2_{\pi^0}$, δM^2_η can turn out negative depending on $\vartheta^\mu_{\pi^+}$, $\vartheta^\mu_{K^+}$, $\vartheta^\mu_{K^0}$. With an appropriate choice of $\vartheta^\mu_{\pi^+}$, $\vartheta^\mu_{K^+}$, $\vartheta^\mu_{K^0}$ (or averaging over randomly chosen twisting angles) we can even suppress the mass corrections as discussed e.g. for nucleons in Ref. [125].

In general, the isospin symmetry is broken in the expressions (2.43). We observe that the breaking occurs in the same way as in the rest frame. The first two components are broken but not the third one. At NLO, pseudoscalar mesons with $I = |I_3|$ remain degenerate and form some multiplet. Charged pions form a duplet with $I = |I_3| = 1$, see Eq. (2.43b). Kaons should form two distinct duplets with $I = |I_3| = 1/2$. However, this is not apparent in Eq. (2.43c). Other pseudoscalar mesons are singlets. Note that the degeneracy among charged and neutral pions is lifted by

$$\delta M^2_{\pi^\pm} - \delta M^2_{\pi^0} = \xi_\pi\left[\mathrm{g}_1(\lambda_\pi) - \mathrm{g}_1(\lambda_\pi, \vartheta_{\pi^+})\right]. \tag{2.44}$$

This splitting term vanishes only for $\vartheta^\mu_{\pi^+} = 0$, namely when the isospin symmetry is restored in the theory. In Ref. [37] a similar splitting term was found using partially quenched ChPT with partially TBC. Analogously, one would expect that a splitting term lifting the degeneracy among kaons. However, at this order no splitting term appears and kaons still remain degenerate, see Eq. (2.43c). The splitting term will appear at NNLO when loop diagrams containing virtual kaons begin to contribute to the mass corrections. In that case the masses of kaons are not degenerate.

The mass corrections of pseudoscalar mesons were recalculated at NLO in Ref. [38]. Therein, the authors adopt a momentum-dependent definition and treat the extra terms $\Delta\vartheta^\mu_{\pi^\pm}$, $\Delta\vartheta^\mu_{K^\pm}$, $\Delta\vartheta^\mu_{K^0}$ as parts of the mass corrections. The results for the neutral pion and the eta meson coincide with Eqs. (2.43a, 2.43d). On the contrary, the results for charged

[6] In Ref. [32], the authors present the corrections of linear masses rather than of squared masses which differ by a factor 1/2.

pions and kaons correspond to Eqs. (2.43b, 2.43c) plus

$$\begin{aligned}&-\frac{2}{M_\pi^2}(p+\vartheta_{\pi^\pm})_\mu\Delta\vartheta^\mu_{\pi^\pm}\\&-\frac{2}{M_K^2}(p+\vartheta_{K^\pm})_\mu\Delta\vartheta^\mu_{K^\pm}\\&-\frac{2}{M_K^2}(p+\vartheta_{K^0})_\mu\Delta\vartheta^\mu_{K^0}.\end{aligned} \tag{2.45}$$

These terms are momentum-dependent and make the mass poles of charged pions and kaons varying. This is not suitable as on lattice the mass is extracted from the exponential of the correlator function evaluated at the pole of the propagator. The pole is, by definition, fixed and momentum-independent otherwise its location would vary as the integration in momentum space is performed further complicating the calculation of the correlator function. Moreover, the terms (2.45) definitely break the isospin symmetry. In general, the three components of the isospin are broken so that pseudoscalar mesons are all singlets. Only in the rest frame, the breaking occurs in the specific way for which pseudoscalar mesons with $I = |I_3|$ remain degenerate.

We remind the reader that at NLO the mass definition of Ref. [36, 37] and the one of Ref. [38] are equivalent. The difference is just formal and lies on which side of Eq. (2.39) the extra terms $\Delta\vartheta^\mu_{\pi^\pm}$ are taken. However, we advocate to adopt the momentum-independent definition [36, 37] as mass poles are at fixed locations as considered in lattice simulations. Furthermore, the expressions (2.43) are more compact and exhibit a degeneracy of pseudoscalar mesons with $I = |I_3|$.

2.3.2 Decay Constants

To determine the corrections of decay constants we consider the matrix elements (1.80) for pions,

$$\mathscr{A}^\mu_{ab} := \langle 0|\, A^\mu_a(0)\, |\phi_b(p)\rangle = i\, p^\mu\, F_{ab}, \qquad a, b = 1, 2, 3. \tag{2.46}$$

According to Ref. [10, 31] the decay constant of the pion is defined as the residue at the mass pole of the two-point function containing the axialvector current and the interpolating field of the pion

$$F_{ab} = \lim_{p^2\to M_\pi^2}(M_\pi^2 - p^2)P_{ab}(p), \tag{2.47}$$

where

$$P_{ab}(p) = N_{\phi_b}\, p_\mu \int \mathrm{d}^4y\; \mathrm{e}^{-i\,py}\, \langle 0|\, T\left\{A^\mu_a(0)\phi_b(y)\right\} |0\rangle\,. \tag{2.48}$$

The prefactor N_{ϕ_b} is a normalization constant which depends on the interpolating field ϕ_b. In finite volume the mass pole as well as the residue are shifted. In Section 2.3.1 we have studied the shift of the mass pole at NLO, see Eqs. (2.35, 2.39). At the same order, the shift of the residue is given by the tadpole diagram of Fig. 1.3b. The diagram looks like that of Fig. 1.2b and generates corrections similar to those of self energies. Evaluating the diagram of pions, we obtain the following two-point functions

$$
\begin{aligned}
P_{\pi^0} &= \frac{N_{\pi^0} p_\mu}{i\left[M_{\pi^0}^2(L) - p^2\right]} \left\{ i p^\mu F_\pi \left[2\Delta B_{\pi^0} + \sqrt{\Delta Z_{\pi^0}}\right] + \mathcal{O}(p^5/F_\pi^3) \right\} \\
P_{\pi^\pm} &= \frac{N_{\pi^\pm}(p+\vartheta_{\pi^\pm})_\mu}{i\left[M_{\pi^\pm}^2(L) - p_{\pi^\pm}^2(L)\right]} \Big\{ i(p+\vartheta_{\pi^\pm})^\mu F_\pi \left[2\Delta B_{\pi^\pm} + \sqrt{\Delta Z_{\pi^\pm}}\right] \\
&\qquad\qquad + 2i\, F_\pi \Delta\vartheta_{\pi^\pm}^\mu + \mathcal{O}(p^5/F_\pi^3) \Big\},
\end{aligned}
\tag{2.49}
$$

where ΔB_{π^0}, $\Delta B_{\pi^\pm}$ are the coefficients of Eqs. (2.27b, 2.28b) and $\Delta\vartheta_{\pi^\pm}^\mu$ are the extra terms of Eq. (2.31). The masses $M_{\pi^0}(L)$, $M_{\pi^\pm}(L)$ are defined so that they are momentum-independent [36,37] and are given by Eqs. (2.35, 2.39). Accordingly, the momentum squares $p_{\pi^\pm}^2(L) = (p + \vartheta_{\pi^\pm} + \Delta\vartheta_{\pi^\pm})^2$ are completed with $\Delta\vartheta_{\pi^\pm}^\mu$ and provide $M_{\pi^\pm}^2(L)$ if external momenta are on the mass shells (2.39). The renormalization constants $\Delta Z_{\pi^0}, \Delta Z_{\pi^\pm}$ are calculated expanding the self energies (2.26) in terms of $(p^0)^2$. At NLO they read

$$
\begin{aligned}
\Delta Z_{\pi^0} &= \frac{1}{1+\Delta B_{\pi^0}} \\
\Delta Z_{\pi^\pm} &= \frac{1}{1+\Delta B_{\pi^\pm}}.
\end{aligned}
\tag{2.50}
$$

Note that in general, the two-point functions P_{π^+}, P_{π^-} are different. In the rest frame, charged pions are degenerate and hence, $P_{\pi^+} = P_{\pi^-}$. This can be showed by similar arguments as those demonstrating $\Delta\Sigma_{\pi^+} = \Delta\Sigma_{\pi^-}$ in the case $p^\mu = \hat{p}^\mu \mathrel{\widehat{=}} \binom{p^0}{\vec{0}}$, see discussion after Eq. (2.34).

To extract the decay constant we must take the residue as in Eq. (2.47). At this order the mass poles in the full propagatores are shifted according to Eqs. (2.35, 2.39). The residues must be then taken in the limits: $p^2 \to M_{\pi^0}^2(L)$ resp. $p_{\pi^\pm}^2(L) \to M_{\pi^\pm}^2(L)$. For the neutral pion, we can take this limit directly and the residue provides

$$
F_{\pi^0}(L) = F_\pi \left[1 + \frac{3}{2}\Delta B_{\pi^0} + \mathcal{O}(p^4/F_\pi^4)\right].
\tag{2.51}
$$

For charged pions the presence of $\Delta\vartheta_{\pi^\pm}^\mu$ additionally shifts the two-point functions $P_{\pi^\pm}$. Contracting the momenta in Eq. (2.49) we obtain two contributions: the first contribution is proportional to $(p+\vartheta_{\pi^\pm})^2\, F_\pi\, [2\Delta B_{\pi^\pm} + \sqrt{\Delta Z_{\pi^\pm}}]$ and the second one is proportional to $2\, F_\pi\, (p+\vartheta_{\pi^\pm})_\mu \Delta\vartheta_{\pi^\pm}^\mu$. In the limits $p_{\pi^\pm}^2(L) \to M_{\pi^\pm}^2(L)$ the momentum squares of the first contribution tend to

$$
(p+\vartheta_{\pi^\pm})^2 \longrightarrow M_{\pi^\pm}^2(L) - 2\,(p+\vartheta_{\pi^\pm})_\mu \Delta\vartheta_{\pi^\pm}^\mu + \mathcal{O}(p^6/F_\pi^4),
\tag{2.52}
$$

due to the on-shell conditions (2.39). Taking the residues, the first contribution then generates a term $\mathcal{O}(p^4/F_\pi)$ which cancels out the second contribution proportional to $2\, F_\pi\, (p+\vartheta_{\pi^\pm})_\mu \Delta\vartheta_{\pi^\pm}^\mu$. At this order the cancellation is exact and we obtain

$$
F_{\pi^\pm}(L) = F_\pi \left[1 + \frac{3}{2}\Delta B_{\pi^\pm} + \mathcal{O}(p^4/F_\pi^4)\right].
\tag{2.53}
$$

The decay constants of other pseudoscalar mesons can be calculated in an analogous way. For the eta meson one proceeds as for the neutral pion. For kaons one follows the derivation of charged pions and takes the residue in a similar way. In that case, a cancellation occurs at $\mathcal{O}(p^4/F_\pi)$ analogous to that described above for $2\,F_\pi\,(p+\vartheta_{\pi^\pm})_\mu \Delta\vartheta^\mu_{\pi^\pm}$. Altogether, the corrections of decay constants read

$$\delta F_{\pi^0} = -\xi_\pi\,\mathrm{g}_1(\lambda_\pi,\vartheta_{\pi^+}) - \frac{\xi_K}{4}\left[\mathrm{g}_1(\lambda_K,\vartheta_{K^+}) + \mathrm{g}_1(\lambda_K,\vartheta_{K^0})\right] \tag{2.54a}$$

$$\delta F_{\pi^\pm} = -\frac{\xi_\pi}{2}\left[\mathrm{g}_1(\lambda_\pi) + \mathrm{g}_1(\lambda_\pi,\vartheta_{\pi^+})\right] - \frac{\xi_K}{4}\left[\mathrm{g}_1(\lambda_K,\vartheta_{K^+}) + \mathrm{g}_1(\lambda_K,\vartheta_{K^0})\right] \tag{2.54b}$$

$$\begin{aligned}\delta F_{K^\pm} = &-\frac{\xi_\pi}{8}\left[\mathrm{g}_1(\lambda_\pi) + 2\,\mathrm{g}_1(\lambda_\pi,\vartheta_{\pi^+})\right] \\ &- \frac{\xi_K}{4}\left[2\,\mathrm{g}_1(\lambda_K,\vartheta_{K^+}) + \mathrm{g}_1(\lambda_K,\vartheta_{K^0})\right] - \frac{3}{8}\xi_\eta\,\mathrm{g}_1(\lambda_\eta)\end{aligned} \tag{2.54c}$$

$$\begin{aligned}\delta F_{K^0} = &-\frac{\xi_\pi}{8}\left[\mathrm{g}_1(\lambda_\pi) + 2\,\mathrm{g}_1(\lambda_\pi,\vartheta_{\pi^+})\right] \\ &- \frac{\xi_K}{4}\left[\mathrm{g}_1(\lambda_K,\vartheta_{K^+}) + 2\,\mathrm{g}_1(\lambda_K,\vartheta_{K^0})\right] - \frac{3}{8}\xi_\eta\,\mathrm{g}_1(\lambda_\eta),\end{aligned} \tag{2.54d}$$

and

$$\delta F_\eta = -\frac{3}{4}\xi_K\left[\mathrm{g}_1(\lambda_K,\vartheta_{K^+}) + \mathrm{g}_1(\lambda_K,\vartheta_{K^0})\right]. \tag{2.54e}$$

The first four expressions coincide with the results of Ref. [36]. As further check we set $\vartheta^\mu_{\pi^+} = \vartheta^\mu_{K^+} = \vartheta^\mu_{K^0} = 0$ and recover the corrections for PBC, see Eqs. (97, 98, 99) of Ref. [32]. At NLO, the dependence on the twist is a phase factor. The sign of overall corrections may change due to the twisting angles and with an appropriate choice of $\vartheta^\mu_{\pi^+}$, $\vartheta^\mu_{K^+}$, $\vartheta^\mu_{K^0}$ (or averaging over randomly chosen twisting angles) we can even suppress the corrections. We observe that the isospin symmetry is broken in the same way as in the rest frame: pseudoscalar mesons with $I = |I_3|$ remain degenerate[7], see Eqs. (2.54b, 2.54c, 2.54d). The splitting term among pions is exactly one half of that for masses (2.44) and has the opposite sign,

$$\delta F_{\pi^\pm} - \delta F_{\pi^0} = \frac{\xi_\pi}{2}\left[\mathrm{g}_1(\lambda_\pi,\vartheta_{\pi^+}) - \mathrm{g}_1(\lambda_\pi)\right]. \tag{2.55}$$

The splitting term among kaons is smaller and originates from loop diagrams containing virtual kaons,

$$\delta F_{K^\pm} - \delta F_{K^0} = \frac{\xi_K}{4}\left[\mathrm{g}_1(\lambda_K,\vartheta_{K^0}) - \mathrm{g}_1(\lambda_K,\vartheta_{K^+})\right]. \tag{2.56}$$

These splitting terms disappear only for $\vartheta^\mu_{\pi^+} = 0$ (or equivalently, $\vartheta^\mu_{K^+} = \vartheta^\mu_{K^0}$) namely when the isospin symmetry is restored in the theory.

The corrections of decay constants were recalculated in Ref. [38]. Therein, the authors define the decay constants directly by the matrix elements $\mathscr{A}^\mu_{ab} = \langle 0|\,A^\mu_a\,|\phi_b\rangle$ in finite volume

[7] At this order the neutral kaon and its antiparticle are degenerate, i.e. $\delta F_{\bar{K}^0} = \delta F_{K^0}$.

and not as the residue of the two-point function (2.48). The results for the neutral pion (resp. the eta meson) with the current A_3^μ (resp. A_8^μ) coincide with Eqs. (2.54a, 2.54e). On the contrary, the results for charged pions and kaons correspond to Eqs. (2.54b, 2.54c, 2.54d) plus terms that in our notation read

$$\begin{aligned}(F^V_{\pi^\pm})^\mu &= 2\,F_\pi \Delta\vartheta^\mu_{\pi^\pm}\\ (F^V_{K^\pm})^\mu &= 2\,F_\pi\,\Delta\vartheta^\mu_{K^\pm}\\ (F^V_{K^0})^\mu &= 2\,F_\pi\,\Delta\vartheta^\mu_{K^0}.\end{aligned} \tag{2.57}$$

These extra terms are the same that appear in the two-point functions, see e.g. Eq. (2.49). In Ref. [38] they are treated as parts of the corrections. Here, we treat them at the same level of the renormalization terms of self energies: they cancel out when the residues of the two-point functions are taken. The decay constants are then defined as the residues and the results do not display the extra terms (2.57). Again, we are faced with two definitions that are equivalent at NLO and just differ formally. However, we advocate to adopt the definition from the residue as it relies on mass poles with fixed locations as considered in lattice simulations. The expressions (2.54) are more compact and exhibit a degeneracy of pseudoscalar mesons with $I = |I_3|$.

2.3.3 Pseudoscalar Coupling Constants

The corrections of the pseudoscalar coupling constants were first calculated in Ref. [38]. Therein, the authors apply the functional method and perform a direct calculation in ChPT with TBC. At NLO the results are

$$\delta G_{\pi^0} = -\frac{\xi_\pi}{2}\,\mathrm{g}_1(\lambda_\pi) - \frac{\xi_K}{4}\,[\mathrm{g}_1(\lambda_K,\vartheta_{K^+}) + \mathrm{g}_1(\lambda_K,\vartheta_{K^0})] - \frac{\xi_\eta}{6}\,\mathrm{g}_1(\lambda_\eta) \tag{2.58a}$$

$$\delta G_{\pi^\pm} = -\frac{\xi_\pi}{2}\,\mathrm{g}_1(\lambda_\pi,\vartheta_{\pi^+}) - \frac{\xi_K}{4}\,[\mathrm{g}_1(\lambda_K,\vartheta_{K^+}) + \mathrm{g}_1(\lambda_K,\vartheta_{K^0})] - \frac{\xi_\eta}{6}\,\mathrm{g}_1(\lambda_\eta) \tag{2.58b}$$

$$\begin{aligned}\delta G_{K^\pm} = &-\frac{\xi_\pi}{8}\,[\mathrm{g}_1(\lambda_\pi) + 2\,\mathrm{g}_1(\lambda_\pi,\vartheta_{\pi^+})]\\ &- \frac{\xi_K}{4}\,[2\,\mathrm{g}_1(\lambda_K,\vartheta_{K^+}) + \mathrm{g}_1(\lambda_K,\vartheta_{K^0})] - \frac{\xi_\eta}{24}\,\mathrm{g}_1(\lambda_\eta)\end{aligned} \tag{2.58c}$$

$$\begin{aligned}\delta G_{K^0} = &-\frac{\xi_\pi}{8}\,[\mathrm{g}_1(\lambda_\pi) + 2\,\mathrm{g}_1(\lambda_\pi,\vartheta_{\pi^+})]\\ &- \frac{\xi_K}{4}\,[\mathrm{g}_1(\lambda_K,\vartheta_{K^+}) + 2\,\mathrm{g}_1(\lambda_K,\vartheta_{K^0})] - \frac{\xi_\eta}{24}\,\mathrm{g}_1(\lambda_\eta)\end{aligned} \tag{2.58d}$$

$$\begin{aligned}\delta G_{\eta} = &-\frac{\xi_\pi}{6}\,[\mathrm{g}_1(\lambda_\pi) + 2\,\mathrm{g}_1(\lambda_\pi,\vartheta_{\pi^+})]\\ &- \frac{\xi_K}{12}\,[\mathrm{g}_1(\lambda_K,\vartheta_{K^+}) + \mathrm{g}_1(\lambda_K,\vartheta_{K^0})] - \frac{\xi_\eta}{2}\,\mathrm{g}_1(\lambda_\eta).\end{aligned} \tag{2.58e}$$

Note that δG_{π^0} (resp. δG_η) correspond to $\Delta^V G_{\pi^0 3}/G_\pi$ (resp. $\Delta^V G_{\eta 8}/G_\eta$) presented in Eq. (6.10) of Ref. [38]. At this order, pseudoscalar mesons with $I = |I_3|$ are degenerate and no extra terms $\Delta\vartheta^{\mu}_{\pi^{\pm}}$, $\Delta\vartheta^{\mu}_{K^{\pm}}$, $\Delta\vartheta^{\mu}_{K^{0}}$ appear in the expressions. We show an alternative way to obtain these results relying on chiral Ward identities.

In finite volume chiral Ward identities are modified by the presence of the twist. If we introduce the twist through the constant vector field v^{μ}_{ϑ} the chiral Ward identities (1.85) become

$$\partial_\mu \langle 0| A^\mu_3(0) \left|\pi^0(p)\right\rangle_L = \hat{m} \langle 0| P_3(0) \left|\pi^0(p)\right\rangle_L \tag{2.59a}$$

$$(\partial - i\vartheta_{\pi^\pm})_\mu \langle 0| A^\mu_{1\mp i2}(0) \left|\pi^\pm(p+\vartheta_{\pi^\pm})\right\rangle_L = \hat{m} \langle 0| P_{1\mp i2}(0) \left|\pi^\pm(p+\vartheta_{\pi^\pm})\right\rangle_L \tag{2.59b}$$

$$(\partial - i\vartheta_{K^\pm})_\mu \langle 0| A^\mu_{4\mp i5}(0) \left|K^\pm(p+\vartheta_{K^\pm})\right\rangle_L = \tfrac{\hat{m}+m_s}{2} \langle 0| P_{4\mp i5}(0) \left|K^\pm(p+\vartheta_{K^\pm})\right\rangle_L \tag{2.59c}$$

$$(\partial - i\vartheta_{K^0})_\mu \langle 0| A^\mu_{6-i7}(0) \left|K^0(p+\vartheta_{K^0})\right\rangle_L = \tfrac{\hat{m}+m_s}{2} \langle 0| P_{6-i7}(0) \left|K^0(p+\vartheta_{K^0})\right\rangle_L \tag{2.59d}$$

$$\begin{aligned}\partial_\mu \langle 0| A^\mu_8(0) \left|\eta(p)\right\rangle_L = {}& \tfrac{\hat{m}+2m_s}{3} \langle 0| P_8(0) \left|\eta(p)\right\rangle_L \\ &+ \sqrt{2}\, \tfrac{\hat{m}-m_s}{3} \langle 0| P_0(0) \left|\eta(p)\right\rangle_L .\end{aligned} \tag{2.59e}$$

Here, the subscript L indicates that the matrix elements are evaluated in finite volume. The external states are given in the physical basis and the operators on the left- (resp. right-) hand side are linear combinations of the axialvector currents (resp. pseudoscalar densities):

$$\begin{aligned} A^\mu_{1\pm i2} &= \frac{1}{\sqrt{2}}(A_1 \pm iA_2)^\mu & P_{1\pm i2} &= \frac{1}{\sqrt{2}}(P_1 \pm iP_2) \\ A^\mu_{4\pm i5} &= \frac{1}{\sqrt{2}}(A_4 \pm iA_5)^\mu & P_{4\pm i5} &= \frac{1}{\sqrt{2}}(P_4 \pm iP_5) \\ A^\mu_{6-i7} &= \frac{1}{\sqrt{2}}(A_6 - iA_7)^\mu & P_{6-i7} &= \frac{1}{\sqrt{2}}(P_6 - iP_7). \end{aligned} \tag{2.60}$$

Note that the chiral Ward identities of charged pions and kaons are shifted by twisting angles. For convenience, we first focus on the identities of pions and show how to determine the corrections of the pseudoscalar coupling constants. The corrections of other pseudoscalar mesons can be determined in an analogous way.

We rewrite the chiral Ward identities of pions as

$$\begin{aligned} \partial_\mu \langle 0| A^\mu_3 \left|\pi^0\right\rangle_L &= \hat{m} \langle 0| P_3 \left|\pi^0\right\rangle_L \\ (\partial - i\vartheta_{\pi^\pm})_\mu \langle 0| A^\mu_{1\mp i2} \left|\pi^\pm\right\rangle_L &= \hat{m} \langle 0| P_{1\mp i2} \left|\pi^\pm\right\rangle_L , \end{aligned} \tag{2.61}$$

and work out both sides of the equations. On the right-hand side the matrix elements are proportional to the pseudoscalar coupling constants in finite volume. At NLO we have

$$\begin{aligned} \hat{m} \langle 0| P_3 \left|\pi^0\right\rangle_L &= \hat{m} G_{\pi^0}(L) \\ \hat{m} \langle 0| P_{1\mp i2} \left|\pi^\pm\right\rangle_L &= \hat{m} G_{\pi^\pm}(L), \end{aligned} \tag{2.62}$$

where we retain terms up to $\mathcal{O}(p^6/F_\pi^3)$. On the left-hand side the matrix elements are proportional to the decay constants in finite volume. Retaining terms up to $\mathcal{O}(p^6/F_\pi^3)$ we have

$$\begin{aligned}\partial_\mu \langle 0| A_3^\mu \left|\pi^0\right\rangle_L &= p^2 F_{\pi^0}(L)\\ (\partial - i\vartheta_{\pi^\pm})_\mu \langle 0| A_{1\mp i2}^\mu \left|\pi^\pm\right\rangle_L &= (p+\vartheta_{\pi^\pm})^2\, F_{\pi^\pm}(L) + 2F_\pi (p+\vartheta_{\pi^\pm})_\mu \Delta\vartheta^\mu_{\pi^\pm}.\end{aligned} \tag{2.63}$$

The pions are on the mass shells and the momentum squares value

$$\begin{aligned}p^2 &= M^2_{\pi^0}(L)\\ (p+\vartheta_{\pi^\pm})^2 &= M^2_{\pi^\pm}(L) - 2(p+\vartheta_{\pi^\pm})_\mu \Delta\vartheta^\mu_{\pi^\pm} + \mathcal{O}(p^6/F_\pi^4).\end{aligned} \tag{2.64}$$

Inserting these expressions in Eq. (2.63) the terms containing $2(p+\vartheta_{\pi^\pm})_\mu\Delta\vartheta^\mu_{\pi^\pm}$ cancel out and we obtain

$$\begin{aligned}\partial_\mu \langle 0| A_3^\mu \left|\pi^0\right\rangle_L &= M^2_{\pi^0}(L) F_{\pi^0}(L)\\ (\partial - i\vartheta_{\pi^\pm})_\mu \langle 0| A_{1\mp i2}^\mu \left|\pi^\pm\right\rangle_L &= M^2_{\pi^\pm}(L) F_{\pi^\pm}(L),\end{aligned} \tag{2.65}$$

where we retain terms up to $\mathcal{O}(p^6/F_\pi^3)$. We equate both sides of the identities and find

$$\begin{aligned}\hat{m} G_{\pi^0}(L) &= M^2_{\pi^0}(L) F_{\pi^0}(L)\\ \hat{m} G_{\pi^\pm}(L) &= M^2_{\pi^\pm}(L)\, F_{\pi^\pm}(L).\end{aligned} \tag{2.66}$$

These relations can be written in terms of finite volume corrections as defined in Eq. (2.42). Dividing both sides for $\hat{m}G_\pi = M_\pi^2 F_\pi$ we find

$$\begin{aligned}\delta G_{\pi^0} &= \delta M^2_{\pi^0} + \delta F_{\pi^0} + \delta M^2_{\pi^0}\, \delta F_{\pi^0}\\ \delta G_{\pi^\pm} &= \delta M^2_{\pi^\pm} + \delta F_{\pi^\pm} + \underbrace{\delta M^2_{\pi^\pm}\, \delta F_{\pi^\pm}}_{\mathcal{O}(\xi_\pi^2)}.\end{aligned} \tag{2.67}$$

Note that the last products are $\mathcal{O}(\xi_\pi^2)$ and go beyond NLO. It turns out that the corrections of the coupling constants are given by the sum of the corrections of the masses and of the decay constants. Inserting the expressions (2.43a, 2.54a, 2.43b, 2.54b) one finds the results (2.58a, 2.58b).

In an analogous way, we determine the corrections of other pseudoscalar mesons. For kaons we obtain,

$$\begin{aligned}\delta G_{K^\pm} &= \delta M^2_{K^\pm} + \delta F_{K^\pm} + \mathcal{O}(\xi_\pi^2)\\ \delta G_{K^0} &= \delta M^2_{K^0} + \delta F_{K^0} + \mathcal{O}(\xi_\pi^2).\end{aligned} \tag{2.68}$$

Inserting (2.43c, 2.54c, 2.54d) one finds the results (2.58c, 2.58d). For the eta meson, we must consider an additional term. From Eq. (2.59e) we see that the chiral Ward identity has term proportional to $\langle 0| P_0(0) \left|\eta(p)\right\rangle_L$. This matrix element can be calculated applying the functional method. In Section 1.4.3 we present the result at NLO in infinite volume, see Eq. (1.87). Here, we give the result at NLO for the difference among the matrix element in finite volume minus the matrix element in infinite volume:

$$\begin{aligned}\Delta G_{0,\eta} &= \langle 0| P_0(0) \left|\eta(p)\right\rangle_L - \langle 0| P_0(0) \left|\eta(p)\right\rangle\\ &= -\frac{\sqrt{2}}{6}\, G_0\, \xi_\pi \left[\mathrm{g}_1(\lambda_\pi) + 2\, \mathrm{g}_1(\lambda_\pi, \vartheta_{\pi^+})\right]\\ &\qquad + \frac{\sqrt{2}}{6}\, G_0 \left\{\xi_K \left[\mathrm{g}_1(\lambda_K, \vartheta_{K^+})) + \mathrm{g}_1(\lambda_K, \vartheta_{K^0})\right] + \xi_\eta\, \mathrm{g}_1(\lambda_\eta)\right\}.\end{aligned} \tag{2.69}$$

Knowing $\Delta G_{0,\eta}$ at NLO we can now proceed as in the case of the neutral pion. Working out both sides of the chiral Ward identity (2.59e) we find a relation connecting the corrections of the pseudoscalar coupling constant with the corrections of the mass, decay constant and $\Delta G_{0,\eta}$:

$$\tfrac{\hat{m}+2m_s}{3} G_\eta \, \delta G_\eta = M_\eta^2 F_\eta \left(\delta M_\eta^2 + \delta F_\eta + \delta M_\eta^2 \, \delta F_\eta \right) - \tfrac{\sqrt{2}}{3} (\hat{m} - m_s) \, \Delta G_{0,\eta}. \tag{2.70}$$

We divide both sides for $\left[\tfrac{\hat{m}+2m_s}{3} G_\eta\right]$ and retain terms relevant at NLO. This gives

$$\delta G_\eta = \delta M_\eta^2 + \delta F_\eta - \frac{\sqrt{2}}{2} \left[\frac{M_\pi^2}{M_\eta^2} - 1 \right] \frac{\Delta G_{0,\eta}}{G_\eta} + \mathcal{O}(\xi_\pi^2). \tag{2.71}$$

Inserting the expressions (2.43d, 2.54e, 2.69) one finds the result (2.58e).

The results (2.58) confirm that at NLO the definitions of Ref. [36, 37] and of Ref. [38] are equivalent. They both respect the chiral Ward identities (2.59). The chiral Ward identities relate the matrix elements in a way that at this order, the renormalization terms of self energies exactly cancel out extra terms arising from the matrix elements of the axialvector decay. This leaves us the choice to treat such terms as parts of the corrections or not. Masses, decay constants and pseudoscalar coupling constants can be then defined accordingly. However, we advocate to adopt the definitions relying on mass poles with fixed locations just as considered on lattice. This avoids further complications in the integration of correlator functions in momentum space.

We add some concluding remarks on the corrections of pseudoscalar coupling constants at NLO. In general, the corrections are negative, see Eq. (2.58). The dependence on the twist is a phase factor and may change the overall sign. The corrections can be even suppressed with an appropriate choice of $\vartheta^\mu_{\pi^+}$, $\vartheta^\mu_{K^+}$, $\vartheta^\mu_{K^0}$ or averaging over randomly chosen twisting angles, see e.g. Ref. [125]. We observe that here, the isospin symmetry is broken in the same way as in the corrections of masses and decay constants: pseudoscalar mesons with $I = |I_3|$ remain degenerate. The splitting term among pions and the one among kaons are exactly as those of decay constants but with the opposite sign,

$$\begin{aligned} \delta G_{\pi^\pm} - \delta G_{\pi^0} &= -\frac{\xi_\pi}{2} \left[\mathrm{g}_1(\lambda_\pi, \vartheta_{\pi^+}) - \mathrm{g}_1(\lambda_\pi) \right] \\ \delta G_{K^\pm} - \delta G_{K^0} &= -\frac{\xi_K}{4} \left[\mathrm{g}_1(\lambda_K, \vartheta_{K^+}) - \mathrm{g}_1(\lambda_K, \vartheta_{K^0}) \right]. \end{aligned} \tag{2.72}$$

These splitting terms disappear for $\vartheta^\mu_{\pi^+} = 0$ (or equivalently, $\vartheta^\mu_{K^+} = \vartheta^\mu_{K^0}$) namely when the isospin symmetry is restored. Setting all twisting angles to zero (i.e. $\vartheta^\mu_{\pi^+} = \vartheta^\mu_{K^+} = \vartheta^\mu_{K^0} = 0$) we obtain,

$$\begin{aligned} \delta G_\pi &= -\frac{\xi_\pi}{2} \, \mathrm{g}_1(\lambda_\pi) - \frac{\xi_K}{2} \, \mathrm{g}_1(\lambda_K) - \frac{\xi_\eta}{6} \, \mathrm{g}_1(\lambda_\eta) \\ \delta G_K &= -\frac{3}{8} \xi_\pi \, \mathrm{g}_1(\lambda_\pi) - \frac{3}{4} \xi_K \, \mathrm{g}_1(\lambda_K) - \frac{\xi_\eta}{24} \, \mathrm{g}_1(\lambda_\eta) \\ \delta G_\eta &= -\frac{\xi_\pi}{2} \, \mathrm{g}_1(\lambda_\pi) - \frac{\xi_K}{6} \, \mathrm{g}_1(\lambda_K) - \frac{\xi_\eta}{2} \, \mathrm{g}_1(\lambda_\eta). \end{aligned} \tag{2.73}$$

These expressions correspond to the corrections of pseudoscalar coupling constants in finite volume with PBC.

2.3.4 Pion Form Factors

To study the finite volume corrections of pion form factors we restrict the group and consider only two light flavors. We impose TBC to QCD and introduce the twist as in Section 2.2 through a constant vector field

$$v^\mu_\vartheta = \vartheta^\mu_3 \frac{\tau_3}{2}. \tag{2.74}$$

Here, τ_3 represents the unique generator of $\mathrm{SU}(2)_V$ commuting with the mass matrix and, at the same time, conserving the electric charge. The twisting angle ϑ^μ_3 shifts the momenta of quark fields. In the effective theory, the momenta of charged pions are shifted by $\vartheta^\mu_{\pi^\pm} = \pm\vartheta^\mu_3$. The corrections of pion masses, decay constants and coupling constants can be calculated as before. One gets

$$\delta M^2_{\pi^0} = \frac{\xi_\pi}{2}\left[2\,\mathrm{g}_1(\lambda_\pi,\vartheta_{\pi^+}) - \mathrm{g}_1(\lambda_\pi)\right] \qquad \delta M^2_{\pi^\pm} = \frac{\xi_\pi}{2}\,\mathrm{g}_1(\lambda_\pi) \tag{2.75a}$$

$$\delta F_{\pi^0} = -\xi_\pi\,\mathrm{g}_1(\lambda_\pi,\vartheta_{\pi^+}) \qquad \delta F_{\pi^\pm} = -\frac{\xi_\pi}{2}\left[\mathrm{g}_1(\lambda_\pi) + \mathrm{g}_1(\lambda_\pi,\vartheta_{\pi^+})\right] \tag{2.75b}$$

$$\delta G_{\pi^0} = -\frac{\xi_\pi}{2}\,\mathrm{g}_1(\lambda_\pi) \qquad \delta G_{\pi^\pm} = -\frac{\xi_\pi}{2}\,\mathrm{g}_1(\lambda_\pi,\vartheta_{\pi^+}). \tag{2.75c}$$

These results can be obtained from Eqs. (2.43, 2.54, 2.58) discarding the contributions of virtual kaons and eta meson. The functions $\mathrm{g}_1(\lambda_\pi)$, $\mathrm{g}_1(\lambda_\pi,\vartheta_{\pi^+})$ are defined in Eqs. (2.9, 2.30) and the parameters λ_π, ξ_π after Eq. (2.9). Note that the restriction to two light flavors implies that the renormalization terms (2.31) become

$$\Delta\vartheta^\mu_{\pi^\pm} = \pm\xi_\pi\,\mathrm{f}^\mu_1(\lambda_\pi,\vartheta_{\pi^+}). \tag{2.76}$$

At NLO the splitting terms among charged and neutral pions remain the same as in the 3-light-flavor case and are given in Eqs. (2.44, 2.55, 2.72).

The corrections of pion form factors can be determined from the matrix elements (1.90). For convenience, we rewrite them as

$$\begin{aligned} \langle\pi_b(p')|\,S_0\,|\pi_a(p)\rangle &= \langle\pi_b|\,S_0\,|\pi_a\rangle \\ \langle\pi_b(p')|\,V^\mu_3\,|\pi_a(p)\rangle &= \langle\pi_b|\,V^\mu_3\,|\pi_a\rangle\,, \end{aligned} \tag{2.77}$$

and define the corrections of the matrix elements as

$$\begin{aligned} \delta\Gamma^{ab}_S &= \frac{\langle\pi_b|\,S_0\,|\pi_a\rangle_L - \langle\pi_b|\,S_0\,|\pi_a\rangle}{\langle\pi_b|\,S_0\,|\pi_a\rangle_{q^2=0}} \\ i(\Delta\Gamma^{ab}_V)^\mu &= \langle\pi_b|\,V^\mu_3\,|\pi_a\rangle_L - \langle\pi_b|\,V^\mu_3\,|\pi_a\rangle\,. \end{aligned} \tag{2.78}$$

Here, the subscript L (resp. $q^2 = 0$) indicates that matrix elements are evaluated in finite volume (resp. in infinite volume at a vanishing momentum transfer).

In finite volume the corrections of form factors still depend on the momentum transfer $q^\mu = (p' - p)^\mu$. The twist shifts the momenta of charged pions but not necessarily induces a continuous q^μ. If the incoming and outgoing pions are the same, the twisting angles cancel out from the spatial components of the momentum transfer and

$$\vec{q} = \left(\vec{p}' + \vec{\vartheta}_{\pi^\pm}\right) - \left(\vec{p} + \vec{\vartheta}_{\pi^\pm}\right) = \frac{2\pi}{L}\vec{l} \qquad \text{with} \qquad \vec{l} \in \mathbb{Z}^3. \tag{2.79}$$

We use this fact to work out the matrix elements and evaluate their corrections. However, we must keep in mind that –depending on the kinematics chosen– the zeroth component q^0 may contain the twisting angles of external pions and hence, vary continuously.

We first discuss the corrections at NLO of the matrix elements of the scalar form factor. The corrections can be evaluated from the loop diagrams of Fig. 1.4 in finite volume. The tadpole diagram generates corrections similar to those encountered in Section 2.3.1. The fish diagram generates additional corrections which can be calculated with the Feynman parametrization (A.4). Altogether, we find

$$\begin{aligned}\delta\Gamma_S^{\pi^0} = {} & \frac{\xi_\pi}{2}\left[2\,\mathrm{g}_1(\lambda_\pi, \vartheta_{\pi^+}) - \mathrm{g}_1(\lambda_\pi)\right] \\ & + \frac{\xi_\pi}{2}\left\{\int_0^1 \mathrm{d}z\, \left[M_\pi^2\, \mathrm{g}_2(\lambda_z, q) + 2\left(q^2 - M_\pi^2\right) \mathrm{g}_2(\lambda_z, q, \vartheta_{\pi^+})\right]\right\} \end{aligned} \tag{2.80a}$$

$$\delta\Gamma_S^{\pi^\pm} = \frac{\xi_\pi}{2}\left\{\mathrm{g}_1(\lambda_\pi) + \int_0^1 \mathrm{d}z\, \left[\left(q^2 - M_\pi^2\right) \mathrm{g}_2(\lambda_z, q) + q^2\, \mathrm{g}_2(\lambda_z, q, \vartheta_{\pi^+})\right]\right\} + P_\mu \Delta\Theta^\mu_{\pi^\pm}. \tag{2.80b}$$

The functions $\mathrm{g}_2(\lambda_z, q, \vartheta), \mathrm{g}_2(\lambda_z, q)$ originate from the fish diagram and can be evaluated by means of the Poisson resummation formula (2.6). We find

$$\begin{aligned}\mathrm{g}_2(\lambda_z, q, \vartheta) &= \frac{2}{M_\pi^2} \sum_{\substack{\vec{n}\in\mathbb{Z}^3 \\ |\vec{n}|\neq 0}} K_0(\lambda_z|\vec{n}|)\ \mathrm{e}^{iL\vec{n}\left[\vec{\vartheta}+\vec{q}(1-z)\right]} \\ \mathrm{g}_2(\lambda_z, q) &= \mathrm{g}_2(\lambda_z, q, 0),\end{aligned} \tag{2.81}$$

with $\lambda_z = \lambda_\pi\sqrt{1 + z(z-1)q^2/M_\pi^2}$. Note that $\mathrm{g}_2(\lambda_z, q, \vartheta)$ is even in the second and third argument. This is a consequence of the discretization of the spatial components of the momentum transfer, see Eq. (2.79). The last term in Eq. (2.80b) consists of the product among

$$P^\mu = (p' + \vartheta_{\pi^\pm})^\mu + (p + \vartheta_{\pi^\pm})^\mu\,, \tag{2.82}$$

and

$$\Delta\Theta^\mu_{\pi^\pm} = \pm\xi_\pi \int_0^1 \mathrm{d}z\, \left[\mathrm{f}_2^\mu(\lambda_z, q, \vartheta_{\pi^+}) + q^\mu\,(1/2 - z)\,\mathrm{g}_2(\lambda_z, q, \vartheta_{\pi^+})\right]. \tag{2.83}$$

The Lorentz vector $\Delta\Theta^\mu_{\pi^\pm}$ has non-vanishing components in the directions where both $\vartheta^\mu_{\pi^\pm}$ and q^μ are non-vanishing. It vanishes for $\vartheta^\mu_{\pi^\pm} = 0$. The function $\mathrm{f}_2^\mu(\lambda_z, q, \vartheta)$ originates from the fish diagram and can be evaluated with the Poisson resummation formula (2.6):

$$\mathrm{f}_2^\mu(\lambda_z, q, \vartheta) = \sum_{\substack{\vec{n}\in\mathbb{Z}^3 \\ |\vec{n}|\neq 0}} \frac{2iL\lambda_z}{\lambda_\pi^2|\vec{n}|}\, n^\mu\, K_1(\lambda_z|\vec{n}|)\ \mathrm{e}^{iL\vec{n}\left[\vec{\vartheta}+\vec{q}(1-z)\right]}. \tag{2.84}$$

Note that as a consequence of the discretization of $\vec{q}$, the function $\mathrm{f}_2^\mu(\lambda_z, q, \vartheta)$ is even in the second argument and odd in the third one.

The corrections (2.80) decay exponentially in $\lambda_\pi = M_\pi L$. In the limit $L \to \infty$ they disappear and hence, one recovers the scalar form factor in infinite volume. As further check we set $\vartheta^\mu_{\pi^\pm} = 0$ and find

$$\delta\Gamma_S = \frac{\xi_\pi}{2}\left[\mathrm{g}_1(\lambda_\pi) + \left[2q^2 - M_\pi^2\right]\int_0^1 \mathrm{d}z\ \mathrm{g}_2(\lambda_z, q)\right]. \tag{2.85}$$

This expression is the result obtained in finite volume with PBC, see Ref. [120, 121]. In this case (i.e. for $\vartheta^\mu_{\pi^\pm} = 0$) the corrections $\delta\Gamma_S$ are negative: the more the volume shrinks the more the value of the scalar form factor decreases. This corresponds to a screening of the scalar charge distribution. The situation can be better understood considering a pion sourrounded by a cloud of virtual particles. The virtual particles have the probability to wind around the finite volume and to be reabsorbed by the pion. The external scalar source has then the probability to probe several times the same virtual particle. This screens the scalar charge distribution of the pion and in finite volume, the value of the scalar form factor decreases.

A screening effect takes place also for small twisting angles. Here, the corrections $\delta\Gamma_S^{\pi^0}$, $\delta\Gamma_S^{\pi^\pm}$ stay negative as the dependence on the twist is roughly a phase factor. The corrections may turn positive for large twisting angles. In that case, antiscreening effects take place. With an appropriate choice of twisting angles we can even suppress the corrections. Note that the terms $P_\mu \Delta\Theta^\mu_{\pi^\pm}$ depend linearly on $\vartheta^\mu_{\pi^\pm}$. This linear dependence increases $\delta\Gamma_S^{\pi^\pm}$ at large twisting angles. Thus, in order to keep the corrections under control, it is important to employ small twisting angles, e.g. $|\vec{\vartheta}_{\pi^\pm}| < \pi/L$.

At a vanishing momentum transfer, the corrections (2.80) reduce to

$$\delta\Gamma_S^{\pi^0}\big|_{q^2=0} = \frac{\xi_\pi}{2}\left\{2\,\mathrm{g}_1(\lambda_\pi, \vartheta_{\pi^+}) - \mathrm{g}_1(\lambda_\pi) + M_\pi^2\left[\mathrm{g}_2(\lambda_\pi) - 2\,\mathrm{g}_2(\lambda_\pi, \vartheta_{\pi^+})\right]\right\} \tag{2.86a}$$

$$\delta\Gamma_S^{\pi^\pm}\big|_{q^2=0} = \frac{\xi_\pi}{2}\left[\mathrm{g}_1(\lambda_\pi) - M_\pi^2\,\mathrm{g}_2(\lambda_\pi)\right] \pm 2\xi_\pi\,(p + \vartheta_{\pi^\pm})_\mu\,\mathrm{f}_2^\mu(\lambda_\pi, \vartheta_{\pi^+}). \tag{2.86b}$$

The new functions are defined setting $q^2 = 0$ in Eqs. (2.81, 2.84) i.e.

$$\mathrm{g}_2(\lambda_\pi, \vartheta_{\pi^+}) = \mathrm{g}_2(\lambda_\pi, 0, \vartheta_{\pi^+}),\quad \mathrm{g}_2(\lambda_\pi) = \mathrm{g}_2(\lambda_\pi, 0, 0),\quad \mathrm{f}_2^\mu(\lambda_\pi, \vartheta_{\pi^+}) = \mathrm{f}_2^\mu(\lambda_\pi, 0, \vartheta_{\pi^+}). \tag{2.87}$$

In Section 1.4.4 we have seen that at a vanishing momentum transfer the Feynman–Hellman Theorem [39, 40] relates the scalar form factor with the derivative of the pion mass, see Eq. (1.94a). This relation can be extended to finite volume. At NLO the relation for the neutral pion reads

$$\delta\Gamma_S^{\pi^0}\big|_{q^2=0} = \frac{\partial}{\partial M_\pi^2}\Delta M_{\pi^0}^2 + \mathcal{O}(M_\pi^4), \tag{2.88}$$

where $\Delta M_{\pi^0}^2 = M_{\pi^0}^2(L) - M_\pi^2$. The relation can be easily showed if one multiplied Eq. (2.75a) with M_π^2 and derive with respect to $\partial_{M_\pi^2} = \partial/\partial M_\pi^2$. The result is Eq. (2.86a).

For charged pions one must make some specification. As pointed out in Ref. [10] the Feynman–Hellman Theorem states that the expectation value $\langle\pi_b|\, S_0\, |\pi_a\rangle_{q^2=0}$ is related to the derivative of the energy level describing the pion eigenstate. In finite volume the energy levels are additionally shifted by the twisting angles and by corrections of the self energies. At NLO the energy levels are given solving Eq. (2.38) with respect to the zeroth component. We obtain

$$E^2_{\pi^\pm}(L) = M_\pi^2 + \left(\vec{p} + \vec{\vartheta}_{\pi^\pm}\right)^2 - \Delta\Sigma_{\pi^\pm} + \mathcal{O}(M_\pi^6). \tag{2.89}$$

Here, $\Delta\Sigma_{\pi^\pm}$ are the self energies (2.26b) and the external momenta are on the mass shells (2.39). Taking the derivative $\partial_{\hat{m}} = \partial/\partial\hat{m}$ on both sides of the equation, the momentum squares $(\vec{p} + \vec{\vartheta}_{\pi^\pm})^2$ disappear. We get

$$\partial_{\hat{m}} E^2_{\pi^\pm}(L) = \partial_{\hat{m}} M_\pi^2 - \partial_{\hat{m}}\Delta\Sigma_{\pi^\pm} + \mathcal{O}(M_\pi^4). \tag{2.90}$$

On the right-hand side, the term $\partial_{\hat{m}} M_\pi^2$ provides the relation of the Feynman–Hellman Theorem in infinite volume, see Eq. (1.94a). Defining the corrections according to Eq. (2.78) and rewriting the remaining terms with $\partial_{\hat{m}} = (\partial M_\pi^2/\partial\hat{m})\, \partial_{M_\pi^2}$, we have

$$\delta\Gamma_S^{\pi^\pm}\big|_{q^2=0} = \frac{\partial}{\partial M_\pi^2}\left[-\Delta\Sigma_{\pi^\pm}\right] + \mathcal{O}(M_\pi^4), \tag{2.91}$$

where the derivative of the self energies is evaluated at $p^2_{\pi^\pm}(L) = M^2_{\pi^\pm}(L)$. This relation extends the statement of the Feynman–Hellman Theorem in finite volume: at $q^2 = 0$ the corrections of the matrix elements of the scalar form factor are related with the derivative of the self energies with the respect to the pion mass. One can show that the expression (2.86b) results deriving Eq. (2.26b) with respect to M_π^2.

The corrections of the matrix element of the vector form factor can be evaluated in a similar way from the loop diagrams of Fig. 1.4. In this case, one must pay attention as the evaluation involves tensors in finite volume. We find

$$\begin{aligned}(\Delta\Gamma_V^{\pi^\pm})^\mu = {} & Q_e\xi_\pi \int_0^1 \mathrm{d}z\, \left\{P^\mu \left[\mathrm{g}_1(\lambda_z, q, \vartheta_{\pi^+}) - \mathrm{g}_1(\lambda_\pi, \vartheta_{\pi^+})\right] + 2P_\nu\, \mathrm{h}_2^{\mu\nu}(\lambda_z, q, \vartheta_{\pi^+})\right\} \\ & - Q_e \left\{\xi_\pi \int_0^1 \mathrm{d}z\, q^\mu\,(1-2z)\left[P_\nu\, \mathrm{f}_2^\nu(\lambda_z, q, \vartheta_{\pi^+})\right] - 2\Delta\vartheta^\mu_{\pi^\pm} + q^2\Delta\Theta^\mu_{\pi^\pm}\right\}.\end{aligned} \tag{2.92}$$

Here, $Q_e = \pm 1$ represents the electric charge of $\pi^\pm$ in elementary units and the new functions are given by

$$\mathrm{g}_1(\lambda_z, q, \vartheta) = \sum_{\substack{\vec{n}\in\mathbb{Z}^3 \\ |\vec{n}|\neq 0}} \frac{4\lambda_z}{\lambda_\pi^2|\vec{n}|}\; K_1(\lambda_z|\vec{n}|)\; \mathrm{e}^{iL\vec{n}\left[\vec{\vartheta}+\vec{q}(1-z)\right]} \tag{2.93a}$$

$$\mathrm{h}_2^{\mu\nu}(\lambda_z, q, \vartheta) = \sum_{\substack{\vec{n}\in\mathbb{Z}^3 \\ |\vec{n}|\neq 0}} \frac{2(\lambda_z)^2}{\lambda_\pi^2|\vec{n}|^2}\, n^\mu n^\nu\, K_2(\lambda_z|\vec{n}|)\; \mathrm{e}^{iL\vec{n}\left[\vec{\vartheta}+\vec{q}(1-z)\right]}. \tag{2.93b}$$

The corrections decay exponentially in $\lambda_\pi = M_\pi L$ and disappear for $L \to \infty$. In Ref. [38] the corrections were calculated in 3-light-flavor ChPT with TBC. Their result coincides with Eq. (2.92) if contributions of virtual kaons and eta meson are discarded. In general, the corrections depend on the twist through a phase factor, see Eq. (2.92). For small twisting angles the corrections stay negative (resp. positive) for positive (resp. negative) pions. This corresponds to a screening of the electric charge distribution. Note that the corrections (2.92) contain terms linear in $\vartheta^\mu_{\pi^\pm}$. This increases the absolute value of $(\Delta\Gamma_V^{\pi^\pm})^\mu$ at large twisting angles.

We set $\vartheta^\mu_{\pi^\pm} = 0$ and compare our expression with results obtained in finite volume with PBC. In this case, we have

$$(\Delta\Gamma_V^{\pi^\pm})^\mu = Q_e \xi_\pi \int_0^1 \mathrm{d}z \ \left\{(p'+p)^\mu \left[\mathrm{g}_1(\lambda_z, q) - \mathrm{g}_1(\lambda_\pi)\right] + 2(p'+p)_\nu \, \mathrm{h}_2^{\mu\nu}(\lambda_z, q)\right\} + 2Q_e\xi_\pi \int_0^1 \mathrm{d}z \ \ z q^\mu \left[(p'+p)_\nu \, \mathrm{f}_2^\nu(\lambda_z, q)\right], \quad (2.94)$$

where new functions are defined setting $\vartheta^\mu = 0$ in Eqs. (2.93a, 2.93b, 2.84) i.e.

$$\mathrm{g}_1(\lambda_z, q) = \mathrm{g}_1(\lambda_z, q, 0), \qquad \mathrm{h}_2^{\mu\nu}(\lambda_z, q) = \mathrm{h}_2^{\mu\nu}(\lambda_z, q, 0), \qquad \mathrm{f}_2^\nu(\lambda_z, q) = \mathrm{f}_2^\nu(\lambda_z, q, 0). \quad (2.95)$$

Our expression coincides with the result obtained by Häfeli [120]. If we consider the zeroth component (i.e. $\mu = 0$) the function $\mathrm{h}_2^{\mu\nu}(\lambda_z, q)$ does not contribute and the corrections (2.94) consists of: one term proportional to $(p'+p)^0$ and one term proportional to q^0. In Ref. [122–124] the corrections are calculated in finite volume with PBC by means of: partially quenched ChPT [122], Lattice regularized ChPT [123] and 3-light-flavor ChPT [124]. The authors present different results for the zeroth component. Although they use different frameworks, we compare their results with Eq. (2.94). In [122, 123] the term proportional to $(p'+p)^0$ is the same as Eq. (2.94) but in [124] is different. The second term (proportional to q^0) differs in all three cases: in [122] this term is absent whereas in [123, 124] two different results are presented and both differ from Eq. (2.94). We make a further comparison and consider Ref. [37]. Therein, the corrections are calculated in partially quenched ChPT with partially TBC. The result is expressed in three distinct contributions: $G_{FV}, G_{FV}^{\mathrm{iso}}, \boldsymbol{G}_{FV}^{\mathrm{rot}}$, see Eq. (19) of [37]. For vanishing twisting angles the contribution G_{FV}^{iso} disappears and the result coincides with the zeroth component of Eq. (2.94). In this sense we agree with [37]. However, we disagree where the authors claim that the contribution $\boldsymbol{G}_{FV}^{\mathrm{rot}}$ disappears when the twisting angles are zero. Actually, such contribution disappears when both the momentum transfer and the twisting angles are zero.

At a vanishing momentum transfer the corrections (2.92) reduce to

$$(\Delta\Gamma_V^{\pi^\pm})^\mu_{q^2=0} = Q_e \left\{4\,\xi_\pi (p + \vartheta_{\pi^\pm})_\nu \, \mathrm{h}_2^{\mu\nu}(\lambda_\pi, \vartheta_{\pi^+}) + 2\,\Delta\vartheta^\mu_{\pi^\pm}\right\}, \quad (2.96)$$

where $\mathrm{h}_2^{\mu\nu}(\lambda_\pi, \vartheta_{\pi^+}) = \mathrm{h}_2^{\mu\nu}(\lambda_\pi, 0, \vartheta_{\pi^+})$. The corrections are non-zero and disappear only for $L \to \infty$. As further check we set $\vartheta^\mu_{\pi^\pm} = 0$: the corrections (2.96) reduce to the result obtained in finite volume with PBC, see Eq. (7) of Ref. [52]. In general, expressions like

Eq. (2.96) indicate that the (electromagnetic) gauge symmetry or Lorentz invariance are broken. In Section 1.4.4 we have seen that at a vanishing momentum transfer the vector form factor equals unity, see Eq. (1.94b). This result follows from the Ward identity [114]. The Ward identity relies on both the gauge symmetry as well as Lorentz invariance and can be derived from the Ward–Takahashi identity [41–43] taking a continuous limit on the momentum transfer. In finite volume the spatial components of the momentum transfer are discrete and the continuous limit can not be taken. The Ward identity is then violated. It turns out that the expressions (2.96) are consequences of the breaking of Lorentz invariance. In Ref. [52] the above considerations are presented for finite volume with PBC. Therein, the authors demonstrate that at a vanishing momentum transfer the corrections respect the gauge symmetry and are a consequence of the breaking of Lorentz invariance. Moreover, they show that the Ward–Takahashi identity holds in finite volume with PBC. In Appendix B we generalize these considerations to our case. In particular, we construct an EFT invariant under gauge transformations which reproduces Eq. (2.96) and show that the Ward–Takahashi identity holds in finite volume with TBC as long as the spatial components of the transfer momentum are discrete.

We make some final remarks on the symmetry properties of the matrix elements of form factors. In Sections 2.3.1—2.3.3 we have seen that the isospin symmetry is broken by twisting angles. In the rest frame, the breaking occurs in a specific way: the first two components are broken but not I_3. Pseudoscalar mesons with $I = |I_3|$ remain degenerate and form some multiplet. We observe that such breaking also occurs in the matrix elements of form factors (2.86, 2.96) if both external pions are in the rest frame (i.e. $\vec{p}\,' = \vec{p} = \vec{0}$). In Sections 2.3.1—2.3.3 we have taken this as a guide line to identify renormalization (or extra) terms $\Delta\vartheta^{\mu}_{\pi^{\pm}}$. The static physical observables (like masses, decay constants or pseudoscalar coupling constants) were defined so that their corrections at NLO still preserve the degeneracy $I = |I_3|$. This can not be done for form factors. In the matrix elements (2.80, 2.92) the isospin symmetry is broken in kinetic (e.g. q^{μ}, P^{μ}) as well as in dynamical quantities (e.g. $\Delta\vartheta^{\mu}_{\pi^{\pm}}$, $\Delta\Theta^{\mu}_{\pi^{\pm}}$). In particular, all functions depending on the zeroth component q^0 already break the degeneracy $I = |I_3|$. It is therefore difficult to identify functions that can be treated as renormalization terms. For this reason, we have not defined form factors in finite volume and we have presented here the corrections of their matrix elements.

To conclude we observe that twisting angles break another symmetry in the form factors. In infinite volume, form factors depend on the square of the momentum transfer and are invariant under rotations of q^{μ}. This rotation invariance corresponds –in position space– to a charge distribution that depends on the radial direction but not on angular ones. In finite volume, the rotation invariance is broken as the matrix elements of form factors depend on products involving the Lorentz vector of winding numbers (i.e. $q_{\mu}n^{\mu}$) and twisting angles (i.e. $q_{\mu}\vartheta^{\mu}_{\pi^{\pm}}$). Hence, the charge distribution is deformed and varies in the angular directions. As a consequence, form factors can not be expanded in powers of q^2. This prevents us to define square radii and curvatures in the way done in Eq. (1.95). In finite volume, new definitions for such quantities are needed, cfr. e.g. Ref. [126–129].

Chapter 3

Asymptotic Formulae

Asymptotic formulae represent another method to estimate finite volume corrections. They relate the corrections of a given physical quantity to an integral of a specific amplitude, evaluated in infinite volume. The method was introduced by Lüscher [22] and relies on a behaviour, universally observed in quantum field theories[1]: for asymptotically large volume the lightest particle of the spectrum provides the dominant contribution to finite volume corrections of physical quantities.

In the hadron sector, the method has been widely applied in combination with ChPT. The result is a collection of asymptotic formulae for pseudoscalar mesons [24–26, 31, 32], nucleons [27–30, 130, 131] and heavy mesons [30]. These formulae are valid in the p-regime and for PBC. Here, we revise the original derivation of the Lüscher formula [23] and show that the method can be generalized to TBC. We derive asymptotic formulae for pseudoscalar mesons and apply them in combination with ChPT. This allows us to estimate corrections beyond NLO in finite volume with TBC.

3.1 Overview of Asymptotic Formulae

In Ref. [22] Lüscher presents an asymptotic formula estimating the mass corrections of a particle P in a finite cubic box with PBC,

$$\begin{aligned}\delta M_P &= \frac{M_P(L) - M_P}{M_P} \\ &= -\frac{6}{2(4\pi)^2\lambda_P}\,\frac{M_\pi}{M_P}\int_{\mathbb{R}} \mathrm{d}y\ \mathrm{e}^{-\lambda_\pi\sqrt{1+y^2}}\,\mathcal{F}_P(iy) + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}}).\end{aligned} \tag{3.1}$$

Here, M_P is the mass of the particle in infinite volume, L is the side length of the cubic box and $\lambda_P = M_P L$. The constant $\bar{\lambda} = \bar{M} L$ contains a mass bound which can be set to $\bar{M} = \sqrt{2}\,M_\pi$, see Ref. [32]. The original Lüscher formula displays an additional term that in Eq. (3.1) is absent as we consider P a pseudoscalar meson. The amplitude $\mathcal{F}_P(iy)$

[1] The theory must have massive fields and small couplings, see Ref. [23].

describes the forward $P\pi$-scattering in infinite volume and is evaluated in Minkowski space. The argument y is a dimensionless real variable so that $\mathcal{F}_P(iy)$ is integrated in a region of the complex plane away from cuts.

In Ref. [31] Colangelo and Häfeli present analogous formulae estimating the corrections of the decay constant F_P and of the pseudoscalar coupling constant G_P,

$$\begin{aligned}
\delta F_P &= \frac{F_P(L) - F_P}{F_P} \\
&= \frac{6}{(4\pi)^2 \lambda_P} \frac{M_\pi}{F_P} \int_{\mathbb{R}} \mathrm{d}y \; \mathrm{e}^{-\lambda_\pi \sqrt{1+y^2}} \mathcal{N}_P(iy) + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}}) \\
\delta G_P &= \frac{G_P(L) - G_P}{G_P} \\
&= \frac{6}{(4\pi)^2 \lambda_P} \frac{M_\pi M_P}{G_P} \int_{\mathbb{R}} \mathrm{d}y \; \mathrm{e}^{-\lambda_\pi \sqrt{1+y^2}} \mathcal{C}_P(iy) + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}}).
\end{aligned} \tag{3.2}$$

The amplitude $\mathcal{N}_P(iy)$ [resp. $\mathcal{C}_P(iy)$] describes the decay in infinite volume of the pseudoscalar meson P in two pions via the axialvector current [resp. the pseudoscalar density]. Both amplitudes are evaluated in Minkowski space and are integrated in a region of the complex plane away from cuts. The amplitudes can be determined evaluating the matrix element $\langle \pi\pi | A_a^\mu | P \rangle$ resp. $\langle \pi\pi | P_a | P \rangle$ in the forward kinematics. In that kinematics, these matrix elements have a pole which does not contribute to the finite volume corrections and must be subtracted. The subtraction can be performed by means of the Taylor expansion: one expands the matrix elements around the mass shell of P and removes the pole which arises in the first term of the expansion, see Ref. [31]. The resulting expressions are analytic and can be integrated in the integration domain of the asymptotic formulae. From such expressions one defines the amplitudes $\mathcal{N}_P(iy)$, $\mathcal{C}_P(iy)$.

The formulae (3.2) are very similar to the Lüscher formula (3.1). They account for the dominant contribution of the finite volume corrections. In this case, the dominant contribution is given by loop diagrams in which exactly one pion propagator is in finite volume. This contribution decays like $\mathcal{O}(\mathrm{e}^{-\lambda_\pi})$ as one can be seen from the integrands of Eqs. (3.1, 3.2). Note that the asymptotic formulae are derived without necessarily relying on ChPT. The explicit form of the effective chiral Lagrangian is never needed in the proof and its knowledge just shortens the derivation [23]. However, for numerical estimations one needs an explicit representation for the amplitudes $\mathcal{F}_P(iy)$, $\mathcal{N}_P(iy)$, $\mathcal{C}_P(iy)$. ChPT provides us with the chiral representation, an analytic representation consistent with low-energy QCD.

In Ref. [116] Colangelo showed that one can resum the asymptotic formulae and improve their accuracy without modifying the original derivation of Lüscher. The resummation accounts for a part of neglected contributions. This part corresponds to the winding numbers $\vec{n} \in \mathbb{Z}^3$ with $|\vec{n}| > 1$. The resummed asymptotic formulae were presented in Ref. [32] and read

$$\delta M_P = -\frac{1}{2(4\pi)^2\lambda_P}\,\frac{M_\pi}{M_P}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\int_{\mathbb{R}}\frac{\mathrm{d}y}{|\vec{n}|}\,\mathrm{e}^{-\lambda_\pi|\vec{n}|\sqrt{1+y^2}}\,\mathcal{F}_P(iy)+\mathcal{O}(\mathrm{e}^{-\bar{\lambda}})$$

$$\delta F_P = \frac{1}{(4\pi)^2\lambda_P}\,\frac{M_\pi}{F_P}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\int_{\mathbb{R}}\frac{\mathrm{d}y}{|\vec{n}|}\,\mathrm{e}^{-\lambda_\pi|\vec{n}|\sqrt{1+y^2}}\,\mathcal{N}_P(iy)+\mathcal{O}(\mathrm{e}^{-\bar{\lambda}}) \tag{3.3}$$

$$\delta G_P = \frac{1}{(4\pi)^2\lambda_P}\,\frac{M_\pi M_P}{G_P}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\int_{\mathbb{R}}\frac{\mathrm{d}y}{|\vec{n}|}\,\mathrm{e}^{-\lambda_\pi|\vec{n}|\sqrt{1+y^2}}\,\mathcal{C}_P(iy)+\mathcal{O}(\mathrm{e}^{-\bar{\lambda}}).$$

For completeness, we have added here the resummed formula for G_P which was not presented in Ref. [32]. The constant $\bar{\lambda} = \bar{M}L$ now contains a larger mass bound which in Ref. [32] was estimated as

$$\bar{M} = \frac{\sqrt{3}+1}{\sqrt{2}}\,M_\pi > \sqrt{3}\,M_\pi. \tag{3.4}$$

Since $\bar{M} > \sqrt{3}\,M_\pi$, the resummed asymptotic formulae account not only for the dominant contribution $\mathcal{O}(\mathrm{e}^{-\lambda_\pi})$ but also for contributions $\mathcal{O}(\mathrm{e}^{-\sqrt{2}\,\lambda_\pi})$ as well as $\mathcal{O}(\mathrm{e}^{-\sqrt{3}\,\lambda_\pi})$. Still, the resummed formulae miss two main classes of contributions [32]:

1. The contributions originating from diagrams with more than one pion propagator in finite volume. In ChPT these contributions are $\mathcal{O}(\mathrm{e}^{-(\sqrt{3}+1)\,\lambda_\pi/\sqrt{2}})$ and start at NNLO.

2. The contributions originating from singularities further away than M_π from the real axis. Such contributions arise if one considers the amplitudes entering the resummed formulae at one loop or if one considers the pion propagator at two (or more) loops. In ChPT these contributions are $\mathcal{O}(\mathrm{e}^{-2\lambda_\pi})$ and show up from NNLO onwards.

The resummed Lüscher formula exactly reproduces the mass corrections at lowest order. This was already noted by Gasser and Leutwyler in Ref. [19,132] where they calculated the mass corrections at NLO with 2-light-flavor ChPT. In fact, if we insert in the asymptotic formulae (3.3) the chiral representation at tree level,

$$\mathcal{F}_\pi(iy) = -\frac{M_\pi^2}{F_\pi^2} \qquad \mathcal{N}_\pi(iy) = -2\,\frac{M_\pi}{F_\pi} \qquad \mathcal{C}_\pi(iy) = -\frac{G_\pi}{F_\pi^2}, \tag{3.5}$$

we obtain dropping $\mathcal{O}(\mathrm{e}^{-\bar{\lambda}})$,

$$\delta M_\pi = \frac{\xi_\pi}{4}\,\mathrm{g}_1(\lambda_\pi) \qquad \delta F_\pi = -\xi_\pi\,\mathrm{g}_1(\lambda_\pi) \qquad \delta G_\pi = -\frac{\xi_\pi}{2}\,\mathrm{g}_1(\lambda_\pi). \tag{3.6}$$

These expressions coincide with the results[2] (2.8, 2.73) if the contributions of virtual kaons and eta meson are discarded. In general, an asymptotic formula –with the corresponding amplitude at l-loop level– provides corrections at $(l+1)$-loop level. Hence, asymptotic formulae automatically push the estimation of the corrections one-loop order higher. In view of this result it would be very convenient to have asymptotic formulae for TBC. On one hand because the twisting angles complicate the calculation of the corrections. On the other hand because up-to-date no corrections beyond the one-loop level has been estimated in finite volume with TBC.

3.2 Asymptotic Formulae for Masses

3.2.1 Preliminary Definitions

We introduce some notation that we will use in the derivation of the asymptotic formulae. We follow Ref. [23] and we work in Euclidean space where $p^\mu = p_\mu = \left[\begin{smallmatrix} p_0 \\ \vec{p} \end{smallmatrix}\right]$, $k^\mu = k_\mu = \left[\begin{smallmatrix} k_0 \\ \vec{k} \end{smallmatrix}\right]$ with $p \cdot k = p_0 k_0 + \vec{p}\,\vec{k}$. We consider a pseudoscalar field $\phi(x)$ describing a spinless particle of the mass M. The propagator of the particle is given by the connected correlation function,

$$\begin{aligned} G(x) &= \langle \phi(x)\phi(0)\rangle \\ &= \int_{\mathbb{R}^4} \frac{\mathrm{d}^4 p}{(2\pi)^4}\, G(p)\, \mathrm{e}^{ipx}. \end{aligned} \tag{3.7}$$

We assume that $G(p)$ has a pole at $p^2 = -M^2$ and no other singularity occurs below the two-particle threshold, i.e. until $p^2 = -4M^2$. We can write

$$G^{-1}(p) = M^2 + p^2 - \Sigma(p), \tag{3.8}$$

where we normalize the self energy so that the propagator has a unit residue,

$$\Sigma(p) = \frac{\partial}{\partial p^\mu}\Sigma(p) = 0 \qquad \text{for} \quad p^2 = -M^2. \tag{3.9}$$

In general, the amputated n-point function $G(p_1, \ldots, p_n)$ is given by the connected correlation function

$$\begin{aligned} \langle \phi(x_1)\ldots\phi(x_n)\rangle = \int_{\mathbb{R}^4} \frac{\mathrm{d}^4 p_1}{(2\pi)^4} \cdots \frac{\mathrm{d}^4 p_n}{(2\pi)^4}\, \mathrm{e}^{i(p_1 x_1 + \cdots + p_n x_n)}\, (2\pi)^4 \delta(p_1 + \cdots + p_n) \\ \times\, G(p_1)\cdots G(p_n)\; G(p_1, \ldots, p_n). \end{aligned} \tag{3.10}$$

For a real $z < 0$ we define

$$G_z(p_1, \ldots, p_n) := G(\tilde{p}_1, \ldots, \tilde{p}_n) \qquad \text{with} \qquad \tilde{p}^\mu = \begin{bmatrix} z\, p_0 \\ \vec{p} \end{bmatrix}. \tag{3.11}$$

[2] In Eq. (2.8a) are given the corrections of squared masses rather than those of linear masses. The two are related as $\delta M_\pi^2 = 2\delta M_\pi + \mathcal{O}$, where $\mathcal{O}$ are contributions beyond the accuracy of asymptotic formulae.

By virtue of the spectral condition one can show that for every fixed configuration $p_1, \ldots, p_n$ of real momenta, $G_z(p_1, \ldots, p_n)$ can be analytically extended in the complex half plane $\mathbb{H} = \{\, z \in \mathbb{C} \mid \mathrm{Re}\, z < 0 \,\}$, see Ref. [23]. Then, the scattering amplitude T results from the mathematical limit

$$T(\vec{p}_1, \vec{p}_2 | \vec{p}_3, \vec{p}_4) = \lim_{\varepsilon \to 0} G_{i-\varepsilon}(p_1, p_2, -p_3, -p_4). \tag{3.12}$$

Here, p_1^μ, p_2^μ (resp. p_3^μ, p_4^μ) are incoming (outgoing) momenta. They are on the mass shell and their zeroth components value

$$p_j^0 = \sqrt{M^2 + |\vec{p}_j|^2} \qquad \text{for} \quad j = 1, \ldots, 4. \tag{3.13}$$

Often, the scattering amplitude is expressed in terms of the three independent Mandelstam variables,

$$\begin{aligned} s &= (p_1 + p_2)^2 = (p_3 + p_4)^2 \\ t &= (p_1 - p_3)^2 = (p_4 - p_2)^2 \\ u &= (p_1 - p_4)^2 = (p_3 - p_2)^2. \end{aligned} \tag{3.14}$$

The sum of the Mandelstam variables coincides with the sum of the squares of the momenta,

$$s + t + u = \sum_{j=1}^{4} p_j^2, \tag{3.15}$$

and here values $s + t + u = -4M^2$ due to the on-shell condition (3.13). Note that the scattering amplitude is invariant under the interchange of the two incoming (or outgoing) particles. This invariance is commonly referred as crossing symmetry and implies

$$T(s, t, u) = T(s, u, t). \tag{3.16}$$

In the Lüscher formula the scattering amplitude enters in the forward kinematics. In that kinematics, initial and final states are equal. In our case, the momenta can be set to $p_1 = p_3 = p$ resp. $p_2 = p_4 = k$ and the Mandelstam variables become

$$\begin{aligned} s &= -2M(M + \nu) \\ t &= 0 \\ u &= -2M(M - \nu). \end{aligned} \tag{3.17}$$

It turns out that the scattering amplitude is a function of a single Lorentz invariant,

$$\begin{aligned} T(\vec{p}, \vec{k} \,|\, \vec{p}, \vec{k}) &= T\big(s(\nu),\, 0,\, u(\nu)\big) \\ &=: \mathcal{F}(\nu), \end{aligned} \tag{3.18}$$

which is called the crossing variable,

$$\nu = \frac{p_0\, k_0 - \vec{p}\,\vec{k}}{M}. \tag{3.19}$$

The amplitude $\mathcal{F}(\nu)$ can be analytically continued in the complex plane, see Fig. 3.1. It has two physical cuts starting at $\nu = \pm M$ and is analytic in the rest of the plane. Owing to the crossing symmetry (3.16) the amplitude $\mathcal{F}(\nu)$ is an even function in ν.

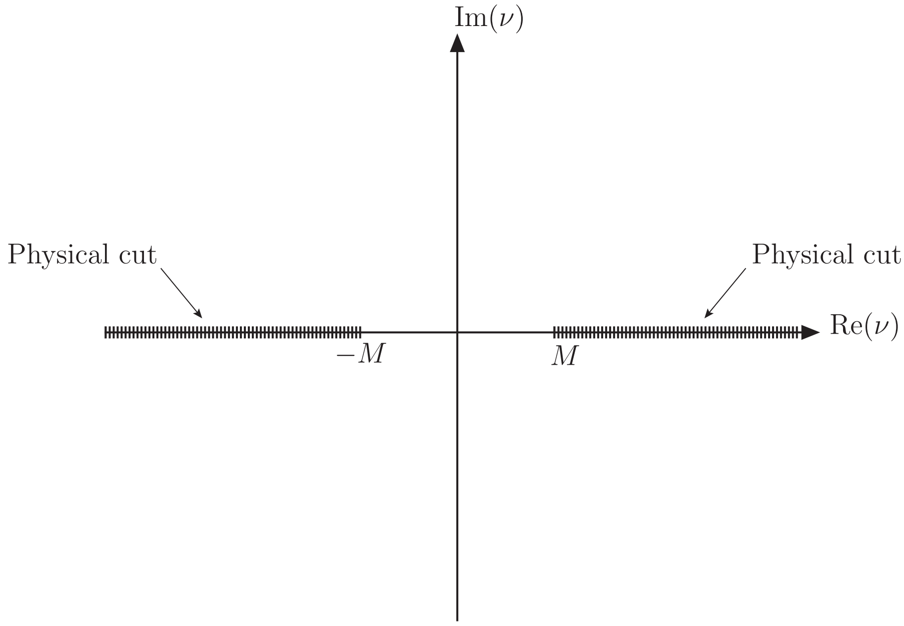


Figure 3.1: Analycity domain of the amplitude $\mathcal{F}(\nu)$ in Minkowski space.

3.2.2 Generalization of the Derivation of Lüscher

In infinite volume the pion propagator reads

$$\begin{aligned} G_\pi(x) &= \int_{\mathbb{R}^4} \frac{\mathrm{d}^4 p}{(2\pi)^4}\, G_\pi(p)\, \mathrm{e}^{ipx} \\ G_\pi^{-1}(p) &= M_\pi^2 + p^2 - \Sigma_\pi(p). \end{aligned} \tag{3.20}$$

Here, we use the convention of Section 3.2.1 and normalize the self energy so that the propagator has a unit residue,

$$\Sigma_\pi(p) = \frac{\partial}{\partial p^\mu}\Sigma_\pi(p) = 0 \qquad \text{for} \quad p^2 = -M_\pi^2. \tag{3.21}$$

The mass M_π is the physical mass of the pion and its expression at NLO in ChPT is given in Eq. (1.78).

Let us consider a cubic box of the side length L on which we impose TBC. We redefine the fields so that they are periodic and we introduce the twist as in Section 2.2. The field redefinition implies that the propagators are periodic in position space. The propagator of the neutral pion becomes

$$\begin{aligned} G_{\pi^0,L}(x) &= \frac{1}{L^3} \sum_{\substack{\vec{p}=\frac{2\pi}{L}\vec{m} \\ \vec{m}\in\mathbb{Z}^3}} \int_{\mathbb{R}} \frac{\mathrm{d}p_0}{2\pi} G_{\pi^0,L}(p)\mathrm{e}^{ipx} \\ G_{\pi^0,L}^{-1}(p) &= M_\pi^2 + p^2 - \Delta\Sigma_{\pi^0}(p), \end{aligned} \tag{3.22}$$

whereas those of charged pions read

$$
\begin{aligned}
G_{\pi^\pm,L}(x) &= \frac{1}{L^3} \sum_{\substack{\vec{p}=\frac{2\pi}{L}\vec{m} \\ \vec{m}\in\mathbb{Z}^3}} \int_{\mathbb{R}} \frac{\mathrm{d}p_0}{2\pi} G_{\pi^\pm,L}(p) \mathrm{e}^{ipx} \\
G^{-1}_{\pi^\pm,L}(p) &= M_\pi^2 + (p+\vartheta_{\pi^\pm})^2 - \Delta\Sigma_{\pi^\pm}(p+\vartheta_{\pi^\pm}).
\end{aligned}
\tag{3.23}
$$

Here, we can leave out the contribution to the self energies in infinite volume as we will later expand in the neighbourhood of the condition (3.21). The twisting angles $\vartheta^\mu_{\pi^\pm}$ are given in Eq. (2.22) and $\Delta\Sigma_{\pi^0}, \Delta\Sigma_{\pi^\pm}$ are normalized so that they just contain the corrections due to finite volume. We expect that $\Delta\Sigma_{\pi^0}, \Delta\Sigma_{\pi^\pm}$ disappear as $L \to \infty$ so that for $\vartheta^\mu_{\pi^\pm} = 0$ the expressions (3.22, 3.23) reduce to the propagator in infinite volume (3.20).

To derive the asymptotic formulae for masses we first consider the pole equation of the neutral pion,

$$
G^{-1}_{\pi^0,L}(p) = M_\pi^2 + p^2 - \Delta\Sigma_{\pi^0}(p) = 0, \qquad \text{for} \quad p^\mu = \begin{bmatrix} iM_{\pi^0}(L) \\ \vec{0} \end{bmatrix}. \tag{3.24}
$$

The momentum p^μ describes the pion at rest in finite volume. We decompose the mass as $M_{\pi^0}(L) = M_\pi + \Delta M_{\pi^0}$ and expand the pole equation around ΔM_{π^0}. Up to quadratic terms we have

$$
\Delta M_{\pi^0} = -\frac{\Delta\Sigma_{\pi^0}(\hat{p})}{2M_\pi + i\left[\frac{\partial}{\partial k^0}\Delta\Sigma_{\pi^0}(k)\right]_{k=\hat{p}}} + \mathcal{O}\big[(\Delta M_{\pi^0})^2\big], \qquad \text{where} \quad \hat{p}^\mu = \begin{bmatrix} iM_\pi \\ \vec{0} \end{bmatrix}. \tag{3.25}
$$

Note that $\hat{p}^\mu$ describes the pion at rest in infinite volume. The above relation is the starting point of the derivation of the asymptotic formula for the mass of the neutral pion.

To derive the asymptotic formula it is necessary to know the asymptotic behaviour of the self energy. In Appendix C we study the asymptotic behaviour of the self energy by means of Abstract Graph Theory. We show that for asymptotically large L the self energy behaves like

$$
\begin{aligned}
\Delta\Sigma_{\pi^0}(\hat{p}) &= \mathcal{O}(\mathrm{e}^{-\frac{\sqrt{3}}{2}\lambda_\pi}) \\
\left[\frac{\partial}{\partial k^0}\Delta\Sigma_{\pi^0}(k)\right]_{k=\hat{p}} &= \mathcal{O}(\mathrm{e}^{-\frac{\sqrt{3}}{2}\lambda_\pi}).
\end{aligned}
\tag{3.26}
$$

By virtue of the asymptotic behaviour, the relation (3.25) may be rewritten as

$$
\Delta M_{\pi^0} = -\frac{\Delta\Sigma_{\pi^0}(\hat{p})}{2M_\pi} + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}}), \tag{3.27}
$$

where $\bar{\lambda} = \bar{M}L$ with $\bar{M} = \sqrt{2}\,M_\pi$, see Appendix C.2. In finite volume, the dominant contribution to the self energy is then given by the diagram of Fig. 3.2. For $P = \pi^0$ we have

$$
\Delta\Sigma_{\pi^0}(\hat{p}) = \frac{I_{\pi^0}}{2} + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}}), \tag{3.28}
$$

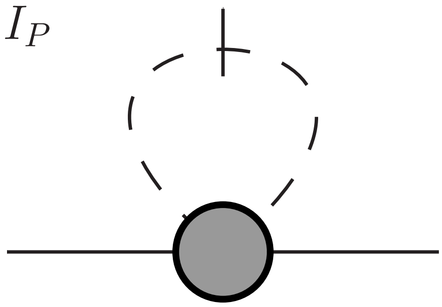


Figure 3.2: Skeleton diagram contributing to asymptotic formulae for masses. Solid lines stand for a generic pseudoscalar meson P and dashed lines for virtual pions. The spline indicates that the pion propagator is in finite volume and accounts for winding numbers $\vec{n} \in \mathbb{Z}^3$ with $|\vec{n}| = 1$. The blob corresponds to the vertex functions defined in the text.

where 1/2 is a symmetry factor and

$$I_{\pi^0} = \sum_{\substack{\vec{n}\in\mathbb{Z}^3 \\ |\vec{n}|=1}} \int_{\mathbb{R}^4} \frac{\mathrm{d}^4 k}{(2\pi)^4} \, \mathrm{e}^{iL\vec{n}\vec{k}} \left[\Gamma_{\pi^0\pi^0} G_\pi(k) + \Gamma_{\pi^0\pi^+} G_\pi(k+\vartheta_{\pi^+}) + \Gamma_{\pi^0\pi^-} G_\pi(k+\vartheta_{\pi^-})\right]. \quad (3.29)$$

The above expression deserves a few comments. The integral I_{π^0} represents the dominant contribution to the self energy. The integral is summed over the winding numbers $\vec{n} \in \mathbb{Z}^3$ with $|\vec{n}| = 1$. Contributions from other winding numbers are $\mathcal{O}(\mathrm{e}^{-\bar{\lambda}})$ and can be neglected. The sum originates from the Poisson resummation formula (2.6). The loop momentum k^μ is continuous and the integrand is multiplied by an exponential factor $\exp(iL\vec{n}\vec{k})$. The exponential factor is responsible for the L-dependence of the entire expression. In the square brackets appear vertex functions and propagators. These quantities are in infinite volume though their momenta are shifted by twisting angles. The vertex functions are defined by the one-particle irreducible part of the amputated four-point function $G(p_1, p_2, p_3, p_4)$, see Ref. [23]. They are analytic and their momentum dependence is

$$\begin{aligned} \Gamma_{\pi^0\pi^0} &= \Gamma_{\pi^0\pi^0}(\hat{p}, k, -k, -\hat{p}) \\ \Gamma_{\pi^0\pi^+} &= \Gamma_{\pi^0\pi^+}(\hat{p}, k+\vartheta_{\pi^+}, -k-\vartheta_{\pi^+}, -\hat{p}) \\ \Gamma_{\pi^0\pi^-} &= \Gamma_{\pi^0\pi^-}(\hat{p}, k+\vartheta_{\pi^-}, -k-\vartheta_{\pi^-}, -\hat{p}), \end{aligned} \quad (3.30)$$

where positive (negative) momenta correspond to incoming (outgoing) pions. The propagators are given by Eq. (3.20). Their momentum dependence is

$$\begin{aligned} G_\pi(k) &= \frac{1}{M_\pi^2 + k^2}, && \text{for virtual } \pi^0, \\ G_\pi(k+\vartheta_{\pi^\pm}) &= \frac{1}{M_\pi^2 + (k+\vartheta_{\pi^\pm})^2}, && \text{for virtual } \pi^\pm. \end{aligned} \quad (3.31)$$

To evaluate the integral I_{π^0} we substitute $k^\mu \mapsto k^\mu - \vartheta^\mu_{\pi^\pm}$ in the expression (3.29). The substitution cancels the twisting angles of virtual pions from the quantities in square brackets and introduces two phase factors,

$$I_{\pi^0} = \sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|=1}} \int_{\mathbb{R}^4} \frac{\mathrm{d}^4 k}{(2\pi)^4}\, \mathrm{e}^{iL\vec{n}\vec{k}}\, G_\pi(k) \left[\Gamma_{\pi^0\pi^0} + \Gamma_{\pi^0\pi^+}\mathrm{e}^{-iL\vec{n}\vec{\vartheta}_{\pi^+}} + \Gamma_{\pi^0\pi^-}\mathrm{e}^{-iL\vec{n}\vec{\vartheta}_{\pi^-}}\right]. \tag{3.32}$$

After the substitution, the vertex functions have all the same momentum dependence,

$$\begin{aligned}\Gamma_{\pi^0\pi^0} &= \Gamma_{\pi^0\pi^0}(\hat{p}, k, -k, -\hat{p})\\ \Gamma_{\pi^0\pi^+} &= \Gamma_{\pi^0\pi^+}(\hat{p}, k, -k, -\hat{p})\\ \Gamma_{\pi^0\pi^-} &= \Gamma_{\pi^0\pi^-}(\hat{p}, k, -k, -\hat{p}).\end{aligned} \tag{3.33}$$

In particular, they depend on three Lorentz scalars: $\hat{p}^2 = -M_\pi^2$, $\hat{p}\cdot k = iM_\pi k_0$ and k^2.

We take a closer look to the expression (3.32). We note that the integration over $\vec{k} = (k_1,\, k_2,\, k_3) \in \mathbb{R}^3$ is independent from spatial rotations: we may replace the exponential factor $\exp(iL\vec{n}\vec{k})$ with $\exp(iL|\vec{n}|k_1)$. The expression can be rewritten as

$$\begin{aligned} I_{\pi^0} &= \int_{\mathbb{R}} \mathrm{d}k_1\, f(k_1)\\ f(k_1) &= \sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|=1}} \int_{\mathbb{R}^3} \frac{\mathrm{d}k_0\ \mathrm{d}^2 k_\perp}{(2\pi)^4}\, \mathrm{e}^{iL|\vec{n}|k_1}\, G_\pi(k) \left[\Gamma_{\pi^0\pi^0} + \Gamma_{\pi^0\pi^+}\mathrm{e}^{-iL\vec{n}\vec{\vartheta}_{\pi^+}} + \Gamma_{\pi^0\pi^-}\mathrm{e}^{-iL\vec{n}\vec{\vartheta}_{\pi^-}}\right],\end{aligned} \tag{3.34}$$

where $k_\perp = (k_2,\, k_3) \in \mathbb{R}^2$. Here, we leave the absolute value $|\vec{n}| = 1$ to track where it enters in the expressions (in this way we can later derive the resummed version of the asymptotic formula). To estimate the integration on k_1 we take the variable k_1 in the complex plane and approximate the integration by the contour of Fig. 3.3. This can be done as the vertex functions are analytic. The integrand $f(k_1)$ has two imaginary poles originating from the denominator of $G_\pi(k)$,

$$k_1^\pm = \pm i\sqrt{M_\pi^2 + k_0^2 + k_\perp^2}. \tag{3.35}$$

The poles depend on $k_0, k_\perp$ and will consequently move when we integrate over those components. We can keep the pole k_1^+ within the contour if we restrict the values of $k_0, k_\perp$ from $\mathbb{R}^3$ to

$$\mathbb{B} = \left\{\ (k_0,\, k_\perp) \in \mathbb{R}^3 \mid k_0^2 + k_\perp^2 \le \frac{5}{4}M_\pi^2\ \right\}. \tag{3.36}$$

Obviously, this restriction affects the result of the k_1-integration but, because of the exponential factor $\exp(iL|\vec{n}|k_1)$ in the integrand $f(k_1)$ and because of

$$\mathrm{Im}(k_1^+) > \frac{3}{2}\, M_\pi > \sqrt{2}\, M_\pi = \bar{M} \qquad \text{for} \quad (k_0,\, k_\perp) \notin \mathbb{B}, \tag{3.37}$$

the net effect is of order $\mathcal{O}(\mathrm{e}^{-\bar{\lambda}})$ and hence, negligible.

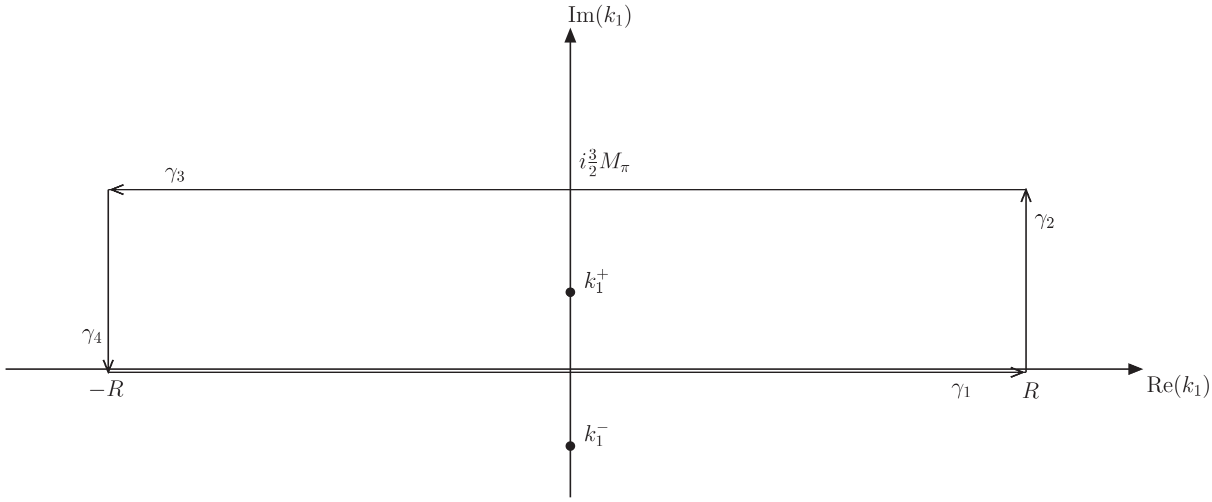


Figure 3.3: Contour for the integration over k_1. Here, $k_1^\pm$ are the poles of $f(k_1)$ and R is a positive real number.

By virtue of the Residue Theorem we may write

$$\int_{\gamma_1} f = 2\pi i\,\mathrm{Res}(f)_{k_1=k_1^+} - \int_{\gamma_2} f - \int_{\gamma_3} f - \int_{\gamma_4} f. \tag{3.38}$$

The integrals on the right-hand side of the equation can be neglected: $\int_{\gamma_2} f$ and $\int_{\gamma_4} f$ vanish as $\frac{1}{\mathrm{Re}(k_1^2)} \sim \frac{1}{R^2}$ for $R \to \infty$ while $\int_{\gamma_3} f \sim \mathcal{O}(\mathrm{e}^{-\bar{\lambda}})$ as $\mathrm{Im}(k_1) = \frac{3}{2}M_\pi > \bar{M}$ along γ_3. The only non-negligible contribution arises from the residue,

$$\begin{aligned}\mathrm{Res}(f)_{k_1=k_1^+} &= \lim_{k_1\to k_1^+}(k_1-k_1^+)f(k_1)\\ &= \sum_{\substack{\vec{n}\in\mathbb{Z}^3\\ |\vec{n}|=1}} \int_{\mathbb{B}} \frac{\mathrm{d}k_0\ \mathrm{d}^2k_\perp}{(2\pi)^4\, 2i|k_1^+|}\, \mathrm{e}^{-L|\vec{n}||k_1^+|}\Big[\Gamma_{\pi^0\pi^0} + \Gamma_{\pi^0\pi^+}\mathrm{e}^{-iL\vec{n}\vec{\vartheta}_{\pi^+}} + \Gamma_{\pi^0\pi^-}\mathrm{e}^{-iL\vec{n}\vec{\vartheta}_{\pi^-}}\Big]_{k_1=k_1^+}.\end{aligned} \tag{3.39}$$

Note that the condition $k_1 = k_1^+$ puts the loop momentum on the mass shell,

$$k^2|_{k_1=k_1^+} = k_0^2 + (k_1^+)^2 + k_\perp^2 = -M_\pi^2. \tag{3.40}$$

Hence, the vertex functions depend on $\hat{p}^2 = -M_\pi^2$, $\hat{p}\cdot k = iM_\pi k_0$ and $k^2 = -M_\pi^2$. We rewrite the integral

$$I_{\pi^0} = \sum_{\substack{\vec{n}\in\mathbb{Z}^3\\ |\vec{n}|=1}} \int_{\mathbb{B}} \frac{\mathrm{d}k_0\ \mathrm{d}^2k_\perp}{2\,(2\pi)^3}\ \frac{e^{-L|\vec{n}|\sqrt{M_\pi^2+k_0^2+k_\perp^2}}}{\sqrt{M_\pi^2+k_0^2+k_\perp^2}}\ \Big[\Gamma_{\pi^0\pi^0} + \Gamma_{\pi^0\pi^+}\mathrm{e}^{-iL\vec{n}\vec{\vartheta}_{\pi^+}} + \Gamma_{\pi^0\pi^-}\mathrm{e}^{-iL\vec{n}\vec{\vartheta}_{\pi^-}}\Big]_{k_1=k_1^+}, \tag{3.41}$$

and we extend the integration on $(k_0,\, k_\perp)$ from $\mathbb{B}$ to $\mathbb{R}^3$. This can be done as the resulting effect is $\mathcal{O}(\mathrm{e}^{-\bar{\lambda}})$. Since the vertex functions are independent from $k_\perp$, we may integrate over $k_\perp$ by means of

$$\int_{\mathbb{R}^2} \frac{\mathrm{d}^2 k_\perp}{(2\pi)^2} \frac{\mathrm{e}^{-\beta\sqrt{\alpha^2+k_\perp^2}}}{2\sqrt{\alpha^2+k_\perp^2}} = \frac{\mathrm{e}^{-\beta\alpha}}{4\pi\beta}. \tag{3.42}$$

The result is

$$I_{\pi^0} = \sum_{\substack{\vec{n}\in\mathbb{Z}^3\\ |\vec{n}|=1}} \int_{\mathbb{R}} \frac{\mathrm{d}k_0}{8\pi^2} \, \frac{\mathrm{e}^{-L|\vec{n}|\sqrt{M_\pi^2+k_0^2}}}{L|\vec{n}|} \left[\Gamma_{\pi^0\pi^0} + (\Gamma_{\pi^0\pi^+} + \Gamma_{\pi^0\pi^-})\,\mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}\right]_{k_1=k_1^+}, \tag{3.43}$$

where we have substituted $\vec{n} \mapsto -\vec{n}$ in the sum and used $\vartheta^\mu_{\pi^-} = -\vartheta^\mu_{\pi^+}$ to reexpress the phase factor with the twisting angle of the negative pion. The expression in the square brackets is on-shell. It corresponds to a forward scattering amplitude in which the neutral pion scatters off neutral and charged pions. The twist enters as a phase factor $\exp(iL\vec{n}\vec{\vartheta}_{\pi^+})$ and gives a different weight to the scattering with charged pions.

From Eqs. (3.27, 3.28, 3.43) we obtain the asymptotic formula for the mass of the neutral pion,

$$\begin{aligned} \delta M_{\pi^0} &= \frac{\Delta M_{\pi^0}}{M_\pi} \\ &= -\frac{1}{2\,(4\pi)^2\,\lambda_\pi} \sum_{\substack{\vec{n}\in\mathbb{Z}^3\\ |\vec{n}|=1}} \int_{\mathbb{R}} \frac{\mathrm{d}y}{|\vec{n}|}\, \mathrm{e}^{-\lambda_\pi|\vec{n}|\sqrt{1+y^2}}\, \mathcal{F}_{\pi^0}(iy, \vartheta_{\pi^+}) + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}}). \end{aligned} \tag{3.44}$$

The amplitude $\mathcal{F}_{\pi^0}(iy, \vartheta_{\pi^+})$ is defined by the forward $\pi\pi$-scattering amplitude weighted by the phase factor containing the twisting angle,

$$\mathcal{F}_{\pi^0}(\tilde{\nu}, \vartheta_{\pi^+}) = T_{\pi^0\pi^0}(0, -4M_\pi\nu) + \left[T_{\pi^0\pi^+}(0, -4M_\pi\nu) + T_{\pi^0\pi^-}(0, -4M_\pi\nu)\right]\mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}. \tag{3.45}$$

Here, $\nu = (s-u)/(4M_\pi)$ corresponds to the crossing variable (3.19) and $\tilde{\nu} = \nu/M_\pi = iy$ is its dimensionless ratio. The functions $T_{\pi^0\pi^0}(t, u-s)$, $T_{\pi^0\pi^+}(t, u-s)$, $T_{\pi^0\pi^-}(t, u-s)$ are the isospin components in infinite volume of the $\pi\pi$-scattering amplitude and in the t-channel with a zero isospin,

$$T^{I=0}_{\pi\pi}(t, u-s) = T_{\pi^0\pi^0}(t, u-s) + T_{\pi^0\pi^+}(t, u-s) + T_{\pi^0\pi^-}(t, u-s), \tag{3.46}$$

see Ref. [32]. They are evaluated in Minkowski space.

The formula (3.44) generalizes the Lüscher formula for pions presented in Eq. (27) of Ref. [22]. It estimates the mass corrections of the neutral pion in finite volume with TBC. The dependence on the twist is given by $\mathcal{F}_{\pi^0}(iy, \vartheta_{\pi^+})$ and namely, by the phase factor $\exp(iL\vec{n}\vec{\vartheta}_{\pi^+})$ contained therein. For $\vartheta^\mu_{\pi^+} = 0$ the phase factor becomes one and the formula (3.44) reduces to the formula valid for PBC and presented by Lüscher in Ref. [22].

The derivation for charged pions involves some complications. The self energies contain renormalization terms that do not enter in the mass definition [36,37] adopted here. These terms must be isolated in order to estimate the mass corrections. In general, we may decompose the self energies in

$$\Delta\Sigma_{\pi^\pm}(p+\vartheta_{\pi^\pm}) = \Delta\bar{\Sigma}_{\pi^\pm} - 2\,(p+\vartheta_{\pi^\pm})\cdot\Delta\vartheta_{\Sigma_{\pi^\pm}} - (\Delta\vartheta_{\Sigma_{\pi^\pm}})^2. \tag{3.47}$$

Here, $\Delta\bar{\Sigma}_{\pi^\pm}$ is defined as the part of the self energies generating the mass corrections and $\Delta\vartheta^\mu_{\Sigma_{\pi^\pm}}$ are the renormalization terms of self energies at higher order[3]. Inserting the decomposition (3.47) in the pole equations we obtain

$$\begin{aligned} G^{-1}_{\pi^\pm,L}(p) &= M_\pi^2 + (p+\vartheta_{\pi^\pm})^2 - \Delta\Sigma_{\pi^\pm}(p+\vartheta_{\pi^\pm}) \\ &= M_\pi^2 + p^2_{\pi^\pm}(L) - \Delta\bar{\Sigma}_{\pi^\pm}, \end{aligned} \tag{3.48}$$

where in the second equality we complete the momentum square $(p+\vartheta_{\pi^\pm})^2$ in similar way as done in Section 2.3.1. The renormalization terms can be reabsorbed in the on-shell conditions which then read $p^2_{\pi^\pm}(L) = (p+\vartheta_{\pi^\pm}+\Delta\vartheta_{\Sigma_{\pi^\pm}})^2 = -M^2_{\pi^\pm}(L)$. Setting $p^2_{\pi^\pm}(L) = -M^2_{\pi^\pm}(L)$ the pole equations (3.48) become equal to zero and define the masses in finite volume. We decompose the masses as $M_{\pi^\pm}(L) = M_\pi + \Delta M_{\pi^\pm}$ and expand the pole equations around $\Delta M_{\pi^\pm}$. Up to quadratic terms we have

$$\Delta M_{\pi^\pm} = -\frac{\Delta\bar{\Sigma}_{\pi^\pm}(p_\pm)}{2M_\pi + i\frac{M_\pi}{\sqrt{M_\pi^2+|\vec{p}_\pm|^2}}\left[\frac{\partial}{\partial k^0}\Delta\bar{\Sigma}_{\pi^\pm}(k)\right]_{k=p_\pm}} + \mathcal{O}\big[(\Delta M_{\pi^\pm})^2\big], \tag{3.49}$$

where

$$p^\mu_\pm = \begin{bmatrix} i\sqrt{M_\pi^2+|\vec{p}_\pm|^2} \\ \vec{p}_\pm \end{bmatrix} \qquad \text{with} \quad \vec{p}_\pm = \vec{p} + \vec{\vartheta}_{\pi^\pm} + \Delta\vec{\vartheta}_{\Sigma_{\pi^\pm}}. \tag{3.50}$$

Note that $p^\mu_\pm$ describe pions on the mass shell of infinite volume despite the presence of twisting angles and renormalization terms in $\vec{p}_\pm$.

To derive the asymptotic formulae for masses we need the asymptotic behaviour of the self energies. In Appendix C we show that for asymptotically large L

$$\begin{aligned} \Delta\Sigma_{\pi^\pm}(p_\pm) &= \mathcal{O}(\mathrm{e}^{-\frac{\sqrt{3}}{2}\lambda_\pi}) \\ \left[\frac{\partial}{\partial k^0}\Delta\Sigma_{\pi^\pm}(k)\right]_{k=p_\pm} &= \mathcal{O}(\mathrm{e}^{-\frac{\sqrt{3}}{2}\lambda_\pi}). \end{aligned} \tag{3.51}$$

[3] In Section 2.3.1 we have calculated these quantities in ChPT at NLO. In Euclidean space, they read

$$\begin{aligned} \Delta\bar{\Sigma}_{\pi^\pm} &= \Delta A_{\pi^\pm} - \Delta B_{\pi^\pm}(p+\vartheta_{\pi^\pm})^2 + \mathcal{O}(p^6/F_\pi^4) \\ \Delta\vartheta^\mu_{\Sigma_{\pi^\pm}} &= \Delta\vartheta^\mu_{\pi^\pm} + \mathcal{O}(p^5/F_\pi^4), \end{aligned}$$

where $\Delta A_{\pi^\pm}$, $\Delta B_{\pi^\pm}$ are given in Eq. (2.28) and $\Delta\vartheta^\mu_{\pi^\pm}$ in Eq. (2.31).

By virtue of the asymptotic behaviour, the relation (3.49) may be rewritten as

$$\begin{aligned}\Delta M_{\pi^\pm} &= -\frac{\Delta\bar{\Sigma}_{\pi^\pm}(p_\pm)}{2M_\pi} + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}}) \\ &= -\frac{\Delta\bar{\Sigma}_{\pi^\pm}(p+\vartheta_{\pi^\pm})}{2M_\pi} + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}}),\end{aligned} \tag{3.52}$$

where $\bar{\lambda} = \bar{M}L$ with $\bar{M} = \sqrt{2}\,M_\pi$, see Appendix C.2. In the last equality of Eq. (3.52) we use the estimate

$$\Delta\bar{\Sigma}_{\pi^\pm}(p_\pm) = \Delta\bar{\Sigma}_{\pi^\pm}(p+\vartheta_{\pi^\pm}) + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}}), \tag{3.53}$$

which follows from the construction of $\Delta\bar{\Sigma}_{\pi^\pm}(p_\pm)$. In general, $\Delta\bar{\Sigma}_{\pi^\pm}(p_\pm)$ is a power series in $(p_\pm)^2$ with coefficients at most $\mathcal{O}(\mathrm{e}^{-\lambda_\pi})$. By definition, $p_\pm^\mu$ contain $\Delta\vec{\vartheta}_{\Sigma_{\pi^\pm}}$, see Eq. (3.50). As $\Delta\vec{\vartheta}_{\Sigma_{\pi^\pm}} \sim \mathcal{O}(\mathrm{e}^{-\lambda_\pi})$ the terms of the power series containing $\Delta\vec{\vartheta}_{\Sigma\pi^\pm}$ are at most $\mathcal{O}(\mathrm{e}^{-2\lambda_\pi})$ and hence, negligible as smaller than $\mathcal{O}(\mathrm{e}^{-\bar{\lambda}})$. This allows us to leave out $\Delta\vec{\vartheta}_{\Sigma\pi^\pm}$ in the argument of $\Delta\bar{\Sigma}_{\pi^\pm}$ and write $(p+\vartheta_{\pi^\pm})^\mu$ at the place of $p_\pm^\mu$.

Without loss of generality, we express Eq. (3.52) as

$$\Delta M_{\pi^\pm} = -\frac{\Delta\bar{\Sigma}_{\pi^\pm}(\hat{p}+\hat{\vartheta}_{\pi^\pm})}{2M_\pi} + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}}), \tag{3.54}$$

where we replace the momenta

$$(p+\vartheta_{\pi^\pm})^\mu = (\hat{p}+\hat{\vartheta}_{\pi^\pm})^\mu, \tag{3.55}$$

with

$$\hat{p}^\mu = \begin{bmatrix} iM_\pi \\ \vec{0} \end{bmatrix}, \qquad \hat{\vartheta}^\mu_{\pi^\pm} = \begin{bmatrix} iD_{\pi^\pm} \\ \vec{\vartheta}_{\pi^\pm} \end{bmatrix}. \tag{3.56}$$

Here, $\hat{p}^\mu$ describes the pion at rest in infinite volume as in Eq. (3.25). The Lorentz vectors $\hat{\vartheta}^\mu_{\pi^\pm}$ have no physical meaning. They depend on the twisting angles of external pions and on the parameters,

$$D_{\pi^\pm} = \sqrt{M_\pi^2 + |\vec{\vartheta}_{\pi^\pm}|^2} - M_\pi. \tag{3.57}$$

Note that such Lorentz vectors disappear when $\vec{\vartheta}_{\pi^\pm} \to \vec{0}$. Later, we make use of this property to perform an expansion in small external twisting angles.

We now estimate the self energies. From Appendix C.2 we know that in finite volume the dominant contribution to the self energies is given by the diagram of Fig. 3.2. Taking into account a symmetry factor 1/2 we have

$$\Delta\Sigma_{\pi^\pm}(\hat{p}+\hat{\vartheta}_{\pi^\pm}) = \frac{I_{\pi^\pm}}{2} + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}}), \tag{3.58}$$

where

$$I_{\pi^\pm} = \sum_{\substack{\vec{n}\in\mathbb{Z}^3 \\ |\vec{n}|=1}} \int_{\mathbb{R}^4} \frac{\mathrm{d}^4k}{(2\pi)^4}\, \mathrm{e}^{iL\vec{n}\vec{k}} \left[\Gamma_{\pi^\pm\pi^0} G_\pi(k) + \Gamma_{\pi^\pm\pi^+} G_\pi(k+\vartheta_{\pi^+}) + \Gamma_{\pi^\pm\pi^-} G_\pi(k+\vartheta_{\pi^-})\right], \tag{3.59}$$

and

$$\begin{aligned}
\Gamma_{\pi^\pm\pi^0} &= \Gamma_{\pi^\pm\pi^0}(\hat{p}+\hat{\vartheta}_{\pi^\pm}, k, -k, -\hat{p}-\hat{\vartheta}_{\pi^\pm}) \\
\Gamma_{\pi^\pm\pi^+} &= \Gamma_{\pi^\pm\pi^+}(\hat{p}+\hat{\vartheta}_{\pi^\pm}, k+\vartheta_{\pi^+}, -k-\vartheta_{\pi^+}, -\hat{p}-\hat{\vartheta}_{\pi^\pm}) \\
\Gamma_{\pi^\pm\pi^-} &= \Gamma_{\pi^\pm\pi^-}(\hat{p}+\hat{\vartheta}_{\pi^\pm}, k+\vartheta_{\pi^-}, -k-\vartheta_{\pi^-}, -\hat{p}-\hat{\vartheta}_{\pi^\pm}).
\end{aligned} \tag{3.60}$$

Vertex functions and propagators are defined as before. To evaluate the integral $I_{\pi^\pm}$ we substitute $k^\mu \mapsto k^\mu - \vartheta^\mu_{\pi^\pm}$ in Eq. (3.59). The substitution cancels the twisting angles of virtual pions from vertex functions as well as from propagators and introduces two phase factors in the integral,

$$I_{\pi^\pm} = \sum_{\substack{\vec{n}\in\mathbb{Z}^3 \\ |\vec{n}|=1}} \int_{\mathbb{R}^4} \frac{\mathrm{d}^4k}{(2\pi)^4}\, \mathrm{e}^{iL\vec{n}\vec{k}} G_\pi(k) \left[\Gamma_{\pi^\pm\pi^0} + \Gamma_{\pi^\pm\pi^+}\mathrm{e}^{-iL\vec{n}\vec{\vartheta}_{\pi^+}} + \Gamma_{\pi^\pm\pi^-}\mathrm{e}^{-iL\vec{n}\vec{\vartheta}_{\pi^-}}\right]. \tag{3.61}$$

Now, the vertex functions have all the same momentum dependence,

$$\begin{aligned}
\Gamma_{\pi^\pm\pi^0} &= \Gamma_{\pi^\pm\pi^0}(\hat{p}+\hat{\vartheta}_{\pi^\pm}, k, -k, -\hat{p}-\hat{\vartheta}_{\pi^\pm}) \\
\Gamma_{\pi^\pm\pi^+} &= \Gamma_{\pi^\pm\pi^+}(\hat{p}+\hat{\vartheta}_{\pi^\pm}, k, -k, -\hat{p}-\hat{\vartheta}_{\pi^\pm}) \\
\Gamma_{\pi^\pm\pi^-} &= \Gamma_{\pi^\pm\pi^-}(\hat{p}+\hat{\vartheta}_{\pi^\pm}, k, -k, -\hat{p}-\hat{\vartheta}_{\pi^\pm}).
\end{aligned} \tag{3.62}$$

Note that the vertex functions still depend on the twisting angles of external pions through the Lorentz vectors $\hat{\vartheta}^\mu_{\pi^\pm}$. We can express the dependence of vertex functions in terms of three Lorentz scalars: $(\hat{p}+\hat{\vartheta}_{\pi^\pm})^2 = -M_\pi^2$, k^2 and $k\cdot(\hat{p}+\hat{\vartheta}_{\pi^\pm})$. Defining

$$\nu_\pm = \frac{k_\mu(\hat{p}+\hat{\vartheta}_{\pi^\pm})^\mu}{M_\pi}, \tag{3.63}$$

we can write

$$\begin{aligned}
\Gamma_{\pi^\pm\pi^0} &= \Gamma_{\pi^\pm\pi^0}(M_\pi^2, k^2, \nu_\pm) \\
\Gamma_{\pi^\pm\pi^+} &= \Gamma_{\pi^\pm\pi^+}(M_\pi^2, k^2, \nu_\pm) \\
\Gamma_{\pi^\pm\pi^-} &= \Gamma_{\pi^\pm\pi^-}(M_\pi^2, k^2, \nu_\pm).
\end{aligned} \tag{3.64}$$

Since twisting angles employed in lattice simulations are preferably small, we may assume that $\hat{\vartheta}^\mu_{\pi^\pm}$ are also small. We expand the vertex functions around $\hat{\vartheta}^\mu_{\pi^\pm} = 0$ or equivalently around $\nu_\pm = \nu$ where by definition, $\nu = k_\mu \hat{p}^\mu / M_\pi$. Up to quadratic terms we have,

$$\Gamma_{\pi^\pm\pi^0} = \Gamma^{(0)}_{\pi^\pm\pi^0}(M_\pi^2, k^2, \nu) + \Gamma^{(1)}_{\pi^\pm\pi^0}(M_\pi^2, k^2, \nu)\, \frac{k_\mu \hat{\vartheta}^\mu_{\pi^\pm}}{M_\pi} + \mathcal{O}\big[(\hat{\vartheta}_{\pi^\pm})^2\big]. \tag{3.65}$$

The functions $\Gamma_{\pi^\pm\pi^+}$, $\Gamma_{\pi^\pm\pi^-}$ have similar expressions. Here, $\Gamma^{(n)}_{\pi^\pm\pi^0}(M_\pi^2, k^2, \nu)$ stands for the n-th derivative in $\nu_\pm$ of the vertex function $\Gamma_{\pi^\pm\pi^0}$, evaluated at $\nu_\pm = \nu$. The expansion (3.65) induces an analogous expansion in powers of $\hat{\vartheta}^\mu_{\pi^\pm}$ in the integral (3.61),

$$I_{\pi^\pm} = I^{(0)}_{\pi^\pm} + I^{(1)}_{\pi^\pm} + \mathcal{O}\big[(\hat{\vartheta}_{\pi^\pm})^2\big]. \tag{3.66}$$

The superscript indicates the derivative order of the vertex functions. The term $I^{(0)}_{\pi^\pm}$ corresponds to the part of the expansion with the zero-th order derivative, namely the integral (3.61) evaluated at $\nu_\pm = \nu$. This integral can be estimated with the contour integration of Fig. 3.3. We proceed as before (see the case of the neutral pion) and find

$$\begin{aligned} I^{(0)}_{\pi^\pm} &= \sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|=1}} \int_{\mathbb{R}^4} \frac{\mathrm{d}^4k}{(2\pi)^4}\, \mathrm{e}^{iL\vec{n}\vec{k}}\, G_\pi(k) \left[\Gamma^{(0)}_{\pi^\pm\pi^0} + \Gamma^{(0)}_{\pi^\pm\pi^+}\mathrm{e}^{-iL\vec{n}\vec{\vartheta}_{\pi^+}} + \Gamma^{(0)}_{\pi^\pm\pi^-}\mathrm{e}^{-iL\vec{n}\vec{\vartheta}_{\pi^-}}\right] \\ &= \sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|=1}} \int_{\mathbb{R}} \frac{\mathrm{d}k_0}{8\pi^2}\, \frac{\mathrm{e}^{-L|\vec{n}|\sqrt{M_\pi^2+k_0^2}}}{L|\vec{n}|} \left[\Gamma^{(0)}_{\pi^\pm\pi^0} + \left(\Gamma^{(0)}_{\pi^\pm\pi^+} + \Gamma^{(0)}_{\pi^\pm\pi^-}\right)\mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}\right]_{k_1=k_1^+} . \end{aligned} \tag{3.67}$$

The second term of Eq. (3.66) contains the part of the expansion with the derivative of the first order,

$$I^{(1)}_{\pi^\pm} = \sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|=1}} \int_{\mathbb{R}^4} \frac{\mathrm{d}^4k}{(2\pi)^4}\, \mathrm{e}^{iL\vec{n}\vec{k}}\, G_\pi(k) \frac{k_\mu \hat{\vartheta}^\mu_{\pi^\pm}}{M_\pi} \left[\Gamma^{(1)}_{\pi^\pm\pi^0} + \Gamma^{(1)}_{\pi^\pm\pi^+}\mathrm{e}^{-iL\vec{n}\vec{\vartheta}_{\pi^+}} + \Gamma^{(1)}_{\pi^\pm\pi^-}\mathrm{e}^{-iL\vec{n}\vec{\vartheta}_{\pi^-}}\right] . \tag{3.68}$$

We decompose this term according to the components of $\hat{\vartheta}^\mu_{\pi^\pm}$,

$$I^{(1)}_{\pi^\pm} = I^{(1)}_{\pi^\pm}\left(\hat{\vartheta}^0_{\pi^\pm}\right) + I^{(1)}_{\pi^\pm}\left(\hat{\vec{\vartheta}}_{\pi^\pm}\right), \tag{3.69}$$

where

$$\begin{aligned} I^{(1)}_{\pi^\pm}\left(\hat{\vartheta}^0_{\pi^\pm}\right) = \sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|=1}} \int_{\mathbb{R}^4} \frac{\mathrm{d}^4k}{(2\pi)^4} \mathrm{e}^{iL\vec{n}\vec{k}} G_\pi(k) \frac{k_0 \hat{\vartheta}^0_{\pi^\pm}}{M_\pi} \\ \times \left[\Gamma^{(1)}_{\pi^\pm\pi^0} + \Gamma^{(1)}_{\pi^\pm\pi^+}\mathrm{e}^{-iL\vec{n}\vec{\vartheta}_{\pi^+}} + \Gamma^{(1)}_{\pi^\pm\pi^-}\mathrm{e}^{-iL\vec{n}\vec{\vartheta}_{\pi^-}}\right], \end{aligned} \tag{3.70a}$$

and

$$\begin{aligned} I^{(1)}_{\pi^\pm}\left(\hat{\vec{\vartheta}}_{\pi^\pm}\right) = -\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|=1}} \int_{\mathbb{R}^4} \frac{\mathrm{d}^4k}{(2\pi)^4} \mathrm{e}^{iL\vec{n}\vec{k}} G_\pi(k) \frac{\vec{k}\hat{\vec{\vartheta}}_{\pi^\pm}}{M_\pi} \\ \times \left[\Gamma^{(1)}_{\pi^\pm\pi^0} + \Gamma^{(1)}_{\pi^\pm\pi^+}\mathrm{e}^{-iL\vec{n}\vec{\vartheta}_{\pi^+}} + \Gamma^{(1)}_{\pi^\pm\pi^-}\mathrm{e}^{-iL\vec{n}\vec{\vartheta}_{\pi^-}}\right] . \end{aligned} \tag{3.70b}$$

To estimate $I^{(1)}_{\pi^\pm}\left(\hat{\vartheta}^0_{\pi^\pm}\right)$ we use the contour of Fig. 3.3 and perform the integration as before. We find

$$\begin{aligned} I^{(1)}_{\pi^\pm}\left(\hat{\vartheta}^0_{\pi^\pm}\right) = \sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|=1}} \int_{\mathbb{R}} \frac{\mathrm{d}k_0}{8\pi^2}\, \frac{k_0 \hat{\vartheta}^0_{\pi^\pm}}{M_\pi}\, \frac{\mathrm{e}^{-L|\vec{n}|\sqrt{M_\pi^2+k_0^2}}}{L|\vec{n}|} \\ \times \left[\Gamma^{(1)}_{\pi^\pm\pi^0} + \left(\Gamma^{(1)}_{\pi^\pm\pi^+} + \Gamma^{(1)}_{\pi^\pm\pi^-}\right)\mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}\right]_{k_1=k_1^+} . \end{aligned} \tag{3.71}$$

The result can be reformulated by means of the chain rule. In the square brackets the derivative with respect to $\nu_\pm$ can be expressed as a derivative in $\nu = k_\mu \hat{p}^\mu / M_\pi = ik_0$. We have

$$I^{(1)}_{\pi^\pm}\big(\hat{\vartheta}^0_{\pi^\pm}\big) = \sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|=1}} \frac{D_{\pi^\pm}}{M_\pi} \int_{\mathbb{R}} \frac{\mathrm{d}k_0}{8\pi^2} \frac{\mathrm{e}^{-L|\vec{n}|\sqrt{M_\pi^2+k_0^2}}}{L|\vec{n}|} \times k_0 \frac{\mathrm{d}}{\mathrm{d}k_0} \Big[\Gamma^{(0)}_{\pi^\pm\pi^0} + \Big(\Gamma^{(0)}_{\pi^\pm\pi^+} + \Gamma^{(0)}_{\pi^\pm\pi^-}\Big)\,\mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}\Big]_{k_1=k_1^+}. \tag{3.72}$$

To estimate $I^{(1)}_{\pi^\pm}\big(\hat{\vec{\vartheta}}_{\pi^\pm}\big)$ we use the differentiation under the integral sign. We introduce a fictitious vector $\vec{x}\in\mathbb{R}^3$ and express the integral in terms of a vectorial function and a gradient in $\vec{x}$ evaluated at $\vec{x} = L\vec{n}$. We have

$$I^{(1)}_{\pi^\pm}\big(\hat{\vec{\vartheta}}_{\pi^\pm}\big) = -\frac{\hat{\vec{\vartheta}}_{\pi^\pm}}{M_\pi} \sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|=1}} \Big[\vec{g}_{\pi^\pm}(\vec{x}) + \vec{\nabla}_{\vec{x}} f_{\pi^\pm}(\vec{x})\Big]_{\vec{x}=L\vec{n}}, \tag{3.73}$$

with

$$\begin{aligned} \vec{g}_{\pi^\pm}(\vec{x}) &= \vec{\vartheta}_{\pi^+} \int_{\mathbb{R}^4} \frac{\mathrm{d}^4k}{(2\pi)^4}\, \mathrm{e}^{i\vec{x}\vec{k}}\, G_\pi(k) \Big[\Gamma^{(1)}_{\pi^\pm\pi^+}\mathrm{e}^{-i\vec{x}\vec{\vartheta}_{\pi^+}} - \Gamma^{(1)}_{\pi^\pm\pi^-}\mathrm{e}^{-i\vec{x}\vec{\vartheta}_{\pi^-}}\Big] \\ f_{\pi^\pm}(\vec{x}) &= \int_{\mathbb{R}^4} \frac{\mathrm{d}^4k}{i\,(2\pi)^4}\, \mathrm{e}^{i\vec{x}\vec{k}}\, G_\pi(k) \Big[\Gamma^{(1)}_{\pi^\pm\pi^0} + \Gamma^{(1)}_{\pi^\pm\pi^+}\mathrm{e}^{-i\vec{x}\vec{\vartheta}_{\pi^+}} + \Gamma^{(1)}_{\pi^\pm\pi^-}\mathrm{e}^{-i\vec{x}\vec{\vartheta}_{\pi^-}}\Big]. \end{aligned} \tag{3.74}$$

The functions $\vec{g}_{\pi^\pm}(\vec{x})$, $f_{\pi^\pm}(\vec{x})$ contain the same kind of integral as before. Using the contour integration of Fig. 3.3 and evaluating the resulting expressions at $\vec{x} = L\vec{n}$, we find

$$I^{(1)}_{\pi^\pm}\big(\hat{\vec{\vartheta}}_{\pi^\pm}\big) = \sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|=1}} \frac{i\vec{n}\hat{\vec{\vartheta}}_{\pi^\pm}}{|\vec{n}|M_\pi} \int_{\mathbb{R}} \frac{\mathrm{d}k_0}{8\pi^2} \frac{\mathrm{e}^{-L|\vec{n}|\sqrt{M_\pi^2+k_0^2}}}{L|\vec{n}|} \left(\frac{1}{L|\vec{n}|} + \sqrt{M_\pi^2+k_0^2}\right) \times \Big[\Gamma^{(1)}_{\pi^\pm\pi^+} - \Gamma^{(1)}_{\pi^\pm\pi^-}\Big]_{k_1=k_1^+} \mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}. \tag{3.75}$$

Again, we express the derivative with respect to $\nu_\pm$ as a derivative in $\nu = ik_0$. This allows us to simplify the expression by means of the partial integration in k_0. We find

$$I^{(1)}_{\pi^\pm}\big(\hat{\vec{\vartheta}}_{\pi^\pm}\big) = \sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|=1}} \frac{\vec{n}\hat{\vec{\vartheta}}_{\pi^\pm}}{|\vec{n}|M_\pi} \int_{\mathbb{R}} \frac{\mathrm{d}k_0}{8\pi^2}\, k_0\, \mathrm{e}^{-L|\vec{n}|\sqrt{M_\pi^2+k_0^2}} \Big[\Gamma^{(0)}_{\pi^\pm\pi^+} - \Gamma^{(0)}_{\pi^\pm\pi^-}\Big]_{k_1=k_1^+} \mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}. \tag{3.76}$$

The results (3.67, 3.72, 3.76) represent the dominant contribution to the self energies $\Delta\Sigma_{\pi^\pm}$. To extract $\Delta\bar{\Sigma}_{\pi^\pm}$ we consider Eq. (3.47) and rewrite the momenta according to Eq. (3.55). The square $(\Delta\vartheta_{\Sigma_{\pi^\pm}})^2$ is $\mathcal{O}(\mathrm{e}^{-2\lambda_\pi})$ and can be neglected. Up to $\mathcal{O}(\mathrm{e}^{-\bar{\lambda}})$ we have

$$\Delta\Sigma_{\pi^\pm}(\hat{p}+\hat{\vartheta}_{\pi^\pm}) = \Delta\bar{\Sigma}_{\pi^\pm} - 2\,\hat{\vec{\vartheta}}_{\pi^\pm}\Delta\vec{\vartheta}_{\Sigma_{\pi^\pm}} + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}}). \tag{3.77}$$

The above expression can be compared to Eq. (3.58) feeded by the expansion (3.66) and by the decomposition (3.69). The comparison yields

$$\Delta\bar{\Sigma}_{\pi^\pm} = \frac{1}{2}\left[I^{(0)}_{\pi^\pm} + I^{(1)}_{\pi^\pm}\big(\hat{\vartheta}^0_{\pi^\pm}\big)\right] + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}}) \tag{3.78a}$$

$$\hat{\vec{\vartheta}}_{\pi^\pm}\Delta\vec{\vartheta}_{\Sigma_{\pi^\pm}} = -\frac{1}{4}\left[I^{(1)}_{\pi^\pm}\big(\hat{\vec{\vartheta}}_{\pi^\pm}\big)\right] + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}}). \tag{3.78b}$$

These identities result from some reasonings based on our knowledge on finite volume effects. In Section 2.3.1 we have seen that the effects generating the mass corrections break the cubic invariance through a phase factor containing the twisting angle of a virtual particle, see e.g. Eq. (2.30). The cubic invariance is broken as long as the twisting angle does not take the value of an integer multiple of $2\pi/L$. An analogous breaking affects Eqs. (3.67, 3.72). For that reason we associate $I^{(0)}_{\pi^\pm}$, $I^{(1)}_{\pi^\pm}\big(\hat{\vartheta}^0_{\pi^\pm}\big)$ to $\Delta\bar{\Sigma}_{\pi^\pm}$. Renormalization terms yield an additional breaking. The cubic invariance is broken not only by phase factors containing twisting angles of virtual particles but also by terms involving the scalar product between the twisting angles of external particles and the winding numbers $\vec{n}$. These terms arise from the contraction of external momenta with vectorial functions such as Eq. (2.33). An analogous breaking affects Eq. (3.76) and therefore we associate $I^{(1)}_{\pi^\pm}\big(\hat{\vec{\vartheta}}_{\pi^\pm}\big)$ to $\Delta\vartheta^\mu_{\Sigma_{\pi^\pm}}$.

From Eqs. (3.54, 3.67, 3.72, 3.78a) we obtain the asymptotic formulae for the masses of charged pions,

$$\begin{aligned}\delta M_{\pi^\pm} &= \frac{\Delta M_{\pi^\pm}}{M_\pi}\\ &= -\frac{1}{2\,(4\pi)^2\,\lambda_\pi}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|=1}}\int_{\mathbb{R}}\frac{\mathrm{d}y}{|\vec{n}|}\,\mathrm{e}^{-\lambda_\pi|\vec{n}|\sqrt{1+y^2}}\\ &\qquad\qquad\times\left(1+y\,\frac{D_{\pi^\pm}}{M_\pi}\frac{\partial}{\partial y}\right)\mathcal{F}_{\pi^\pm}(iy,\vartheta_{\pi^+}) + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}}).\end{aligned} \tag{3.79}$$

The amplitudes are defined by the forward $\pi\pi$-scattering amplitude weighted by a phase factor,

$$\mathcal{F}_{\pi^\pm}(\tilde{\nu},\vartheta_{\pi^+}) = T_{\pi^\pm\pi^0}(0,-4M_\pi\nu) + \left[T_{\pi^\pm\pi^+}(0,-4M_\pi\nu) + T_{\pi^\pm\pi^-}(0,-4M_\pi\nu)\right]\mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}. \tag{3.80}$$

Here, $T_{\pi^\pm\pi^0}(t,u-s)$, $T_{\pi^\pm\pi^+}(t,u-s)$, $T_{\pi^\pm\pi^-}(t,u-s)$ are the isospin components in infinite volume of the $\pi\pi$-scattering amplitude in the t-channel with a zero isospin,

$$T^{I=0}_{\pi\pi}(t,u-s) = T_{\pi^\pm\pi^0}(t,u-s) + T_{\pi^\pm\pi^+}(t,u-s) + T_{\pi^\pm\pi^-}(t,u-s), \tag{3.81}$$

see Ref. [32]. They are evaluated in Minkowski space.

The asymptotic formulae (3.79) generalize the Lüscher formula for pions presented in Ref. [22]. They estimate the mass corrections of charged pions in finite volume with TBC. The dependence on the twist is twofold. On one hand, the formulae depend on the twisting angle of the virtual positive pion through the phase factor $\exp(iL\vec{n}\vec{\vartheta}_{\pi^+})$ contained in the amplitudes. On the other hand, the formulae depend on the twisting angles of external pions through the parameters $D_{\pi^\pm}$, see Eq. (3.57). If we set all twisting angles to zero we recover the formula valid for PBC and presented by Lüscher in Ref. [22]. Note that the dependence on external twisting angles is a consequence of the expansion (3.65). Indeed, the formulae (3.79) represent the first terms of an expansion in powers of $D_{\pi^\pm}$ whose validity relies on the smallness of external twisting angles.

The asymptotic formulae for the masses of other pseudoscalar mesons can be derived in an analogous way. For the eta meson we proceed as for the neutral pion. For kaons we follow the derivation of charged pions and isolate the part of the self energies generating the mass corrections. Altogether, we find

$$\begin{aligned}\delta M_{K^\pm} = &-\frac{1}{2\,(4\pi)^2\,\lambda_K}\frac{M_\pi}{M_K}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|=1}}\int_{\mathbb{R}}\frac{\mathrm{d}y}{|\vec{n}|}\,\mathrm{e}^{-\lambda_\pi|\vec{n}|\sqrt{1+y^2}}\\ &\times\left(1+y\,\frac{D_{K^\pm}}{M_K}\frac{\partial}{\partial y}\right)\mathcal{F}_{K^\pm}(iy,\vartheta_{\pi^+})+\mathcal{O}(\mathrm{e}^{-\bar{\lambda}})\end{aligned} \tag{3.82a}$$

$$\begin{aligned}\delta M_{K^0} = &-\frac{1}{2\,(4\pi)^2\,\lambda_K}\frac{M_\pi}{M_K}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|=1}}\int_{\mathbb{R}}\frac{\mathrm{d}y}{|\vec{n}|}\,\mathrm{e}^{-\lambda_\pi|\vec{n}|\sqrt{1+y^2}}\\ &\times\left(1+y\,\frac{D_{K^0}}{M_K}\frac{\partial}{\partial y}\right)\mathcal{F}_{K^0}(iy,\vartheta_{\pi^+})+\mathcal{O}(\mathrm{e}^{-\bar{\lambda}})\end{aligned} \tag{3.82b}$$

$$\delta M_\eta = -\frac{1}{2\,(4\pi)^2\,\lambda_\eta}\frac{M_\pi}{M_\eta}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|=1}}\int_{\mathbb{R}}\frac{\mathrm{d}y}{|\vec{n}|}\,\mathrm{e}^{-\lambda_\pi|\vec{n}|\sqrt{1+y^2}}\,\mathcal{F}_\eta(iy,\vartheta_{\pi^+})+\mathcal{O}(\mathrm{e}^{-\bar{\lambda}}), \tag{3.82c}$$

where

$$D_{K^\pm} = \sqrt{M_K^2+|\vec{\vartheta}_{K^\pm}|^2}-M_K \qquad D_{K^0} = \sqrt{M_K^2+|\vec{\vartheta}_{K^0}|^2}-M_K. \tag{3.83}$$

The amplitudes $\mathcal{F}_{K^\pm}(iy,\vartheta_{\pi^+})$, $\mathcal{F}_{K^0}(iy,\vartheta_{\pi^+})$ are defined through the forward $K\pi$-scattering amplitude,

$$\begin{aligned}\mathcal{F}_{K^\pm}(\tilde{\nu},\vartheta_{\pi^+}) &= T_{K^\pm\pi^0}(0,-4M_K\nu)\\ &\quad+\left[T_{K^\pm\pi^+}(0,-4M_K\nu)+T_{K^\pm\pi^-}(0,-4M_K\nu)\right]\mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}\\ \mathcal{F}_{K^0}(\tilde{\nu},\vartheta_{\pi^+}) &= T_{K^0\pi^0}(0,-4M_K\nu)\\ &\quad+\left[T_{K^0\pi^+}(0,-4M_K\nu)+T_{K^0\pi^-}(0,-4M_K\nu)\right]\mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}.\end{aligned} \tag{3.84}$$

Here, $\nu = (s-u)/(4M_K)$ is the crossing variable of the $K\pi$-scattering and $\tilde{\nu} = \nu/M_\pi = iy$. The functions $T_{K^\pm\pi^0}(t, u-s), \ldots, T_{K^0\pi^-}(t, u-s)$ are the isospin components in infinite volume of the $K\pi$-scattering amplitude in the t-channel with a zero isospin,

$$\begin{aligned} T_{K\pi}^{I=0}(t, u-s) &= T_{K^\pm\pi^0}(t, u-s) + T_{K^\pm\pi^+}(t, u-s) + T_{K^\pm\pi^-}(t, u-s) \\ &= T_{K^0\pi^0}(t, u-s) + T_{K^0\pi^+}(t, u-s) + T_{K^0\pi^-}(t, u-s), \end{aligned} \tag{3.85}$$

see Ref. [32]. They are evaluated in Minkowski space.

The amplitude $\mathcal{F}_\eta(iy, \vartheta_{\pi^+})$ is defined through the forward $\eta\pi$-scattering amplitude in a similar way,

$$\mathcal{F}_\eta(\tilde{\nu}, \vartheta_{\pi^+}) = T_{\eta\pi^0}(0, -4M_\eta\nu) + \left[T_{\eta\pi^+}(0, -4M_\eta\nu) + T_{\eta\pi^-}(0, -4M_\eta\nu)\right] \mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}, \tag{3.86}$$

where $\nu = (s-u)/(4M_\eta)$ and $\tilde{\nu} = \nu/M_\pi = iy$. The functions $T_{\eta\pi^0}(t, u-s)$, $T_{\eta\pi^+}(t, u-s)$, $T_{\eta\pi^-}(t, u-s)$ are the isospin components in infinite volume of the $\eta\pi$-scattering amplitude in the t-channel with a zero isospin,

$$T_{\eta\pi}^{I=0}(t, u-s) = T_{\eta\pi^0}(t, u-s) + T_{\eta\pi^+}(t, u-s) + T_{\eta\pi^-}(t, u-s), \tag{3.87}$$

see Ref. [32]. The formulae (3.82) generalize the formulae presented in Eq. (22) of Ref. [32]. They depend on the twisting angle of the virtual positive pion through the phase factor $\exp(iL\vec{n}\vec{\vartheta}_{\pi^+})$. The formulae for kaons additionally depend on the external twisting angles of kaons through the parameters $D_{K^\pm}$, D_{K^0}. These formulae result from expansions similar to Eq. (3.65) and are valid for small external twisting angles. Note that if all twisting angles are set to zero the formulae (3.82) reduce to the formulae valid for PBC and presented in Ref. [32].

3.2.3 Asymptotic Formulae for Renormalization Terms and Resummation

The derivation of Section 3.2.2 provides us not only with asymptotic formulae for the masses but also with asymptotic formulae for the renormalization terms of the self energies. For instance, we can derive asymptotic formulae for $\Delta\vartheta^\mu_{\Sigma_{\pi^\pm}}$ from the identities (3.78b) inserting the expressions (3.76). Altogether, we obtain

$$\Delta\vec{\vartheta}_{\Sigma_{\pi^\pm}} = -\frac{M_\pi}{2\,(4\pi)^2} \sum_{\substack{\vec{n}\in\mathbb{Z}^3 \\ |\vec{n}|=1}} \frac{\vec{n}}{|\vec{n}|} \int_{\mathbb{R}} \mathrm{d}y\ \mathrm{e}^{-\lambda_\pi|\vec{n}|\sqrt{1+y^2}}\ y\ \mathcal{G}_{\pi^\pm}(iy, \vartheta_{\pi^+}) + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}}) \tag{3.88a}$$

$$\Delta\vec{\vartheta}_{\Sigma_{K^\pm}} = -\frac{1}{2\,(4\pi)^2} \frac{M_\pi^2}{M_K} \sum_{\substack{\vec{n}\in\mathbb{Z}^3 \\ |\vec{n}|=1}} \frac{\vec{n}}{|\vec{n}|} \int_{\mathbb{R}} \mathrm{d}y\ \mathrm{e}^{-\lambda_\pi|\vec{n}|\sqrt{1+y^2}}\ y\ \mathcal{G}_{K^\pm}(iy, \vartheta_{\pi^+}) + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}}) \tag{3.88b}$$

$$\Delta\vec{\vartheta}_{\Sigma_{K^0}} = -\frac{1}{2\,(4\pi)^2} \frac{M_\pi^2}{M_K} \sum_{\substack{\vec{n}\in\mathbb{Z}^3 \\ |\vec{n}|=1}} \frac{\vec{n}}{|\vec{n}|} \int_{\mathbb{R}} \mathrm{d}y\ \mathrm{e}^{-\lambda_\pi|\vec{n}|\sqrt{1+y^2}}\ y\ \mathcal{G}_{K^0}(iy, \vartheta_{\pi^+}) + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}}). \tag{3.88c}$$

The amplitudes are defined by the difference of the isospin components,

$$\mathcal{G}_{\pi^\pm}(\tilde{\nu},\vartheta_{\pi^+}) = \left[T_{\pi^\pm\pi^+}(0,-4M_\pi\nu) - T_{\pi^\pm\pi^-}(0,-4M_\pi\nu)\right] \mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}} \tag{3.89a}$$

$$\mathcal{G}_{K^\pm}(\tilde{\nu},\vartheta_{\pi^+}) = \left[T_{K^\pm\pi^+}(0,-4M_K\nu) - T_{K^\pm\pi^-}(0,-4M_K\nu)\right] \mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}} \tag{3.89b}$$

$$\mathcal{G}_{K^0}(\tilde{\nu},\vartheta_{\pi^+}) = \left[T_{K^0\pi^+}(0,-4M_K\nu) - T_{K^0\pi^-}(0,-4M_K\nu)\right] \mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}. \tag{3.89c}$$

The asymptotic formulae for the renormalization terms are valid for small external twisting angles. They depend on the twist through the phase factor $\exp(iL\vec{n}\vec{\vartheta}_{\pi^+})$ contained in the amplitudes. Note that for $\vartheta^\mu_{\pi^+}=0$ the sums in Eq. (3.88) are odd in $\vec{n}$ and hence, disappear. This is in accordance with the expectation that renormalization terms are not present in finite volume with PBC.

Until now, we have derived asymptotic formulae accounting only for winding numbers $\vec{n}\in\mathbb{Z}^3$ with $|\vec{n}|=1$. These winding numbers provide the dominant contribution to finite volume corrections and originate from loop diagrams in which exactly one pion propagator is in finite volume. In those cases, virtual pions can propagate over the length $L|\vec{n}|=L$ and wind around the volume exactly once. Obviously, there are virtual pions which can propagate further and wind around the volume more than once. We may include the contribution of such pions in a very simple way, see Ref. [116]. We must replace $|\vec{n}|=1$ with $|\vec{n}|\neq 0$ in all sums of the derivation of Section 3.2.2. As pointed out in Ref. [116] this resummation is of the same nature as the extension of the integration from $\mathbb{B}$ to $\mathbb{R}^3$ done after Eq. (3.41) and does not modify the arguments of the derivation. It turns out that the numerical accuracy of the asymptotic formulae is improved since contributions $\mathcal{O}(\mathrm{e}^{-\sqrt{2}\lambda_\pi})$ and $\mathcal{O}(\mathrm{e}^{-\sqrt{3}\lambda_\pi})$ are now taken into account near to the dominant one. As illustrative example, we write down the resummed asymptotic formulae for pion masses,

$$\begin{aligned}
\delta M_{\pi^0} &= -\frac{1}{2\,(4\pi)^2\,\lambda_\pi}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\int_{\mathbb{R}}\frac{\mathrm{d}y}{|\vec{n}|}\,\mathrm{e}^{-\lambda_\pi|\vec{n}|\sqrt{1+y^2}}\,\mathcal{F}_{\pi^0}(iy,\vartheta_{\pi^+})+\mathcal{O}(\mathrm{e}^{-\bar{\lambda}})\\
\delta M_{\pi^\pm} &= -\frac{1}{2\,(4\pi)^2\,\lambda_\pi}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\int_{\mathbb{R}}\frac{\mathrm{d}y}{|\vec{n}|}\,\mathrm{e}^{-\lambda_\pi|\vec{n}|\sqrt{1+y^2}}\\
&\qquad\times\left(1+y\,\frac{D_{\pi^\pm}}{M_\pi}\frac{\partial}{\partial y}\right)\mathcal{F}_{\pi^\pm}(iy,\vartheta_{\pi^+})+\mathcal{O}(\mathrm{e}^{-\bar{\lambda}}).
\end{aligned} \tag{3.90}$$

Note that the sums run over $\vec{n}\in\mathbb{Z}^3$ with $|\vec{n}|\neq 0$ and the constant $\bar{\lambda}=\bar{M}L$ contains the mass bound $\bar{M}=(\sqrt{3}+1)\,M_\pi/\sqrt{2}$, given in Eq. (3.4).

We apply the resummed asymptotic formulae at lowest order in combination with

ChPT. We insert the chiral representation at tree level,

$$
\begin{aligned}
\mathcal{F}_{\pi^0}(\tilde{\nu},\vartheta_{\pi^+}) &= \frac{M_\pi^2}{F_\pi^2}\left(1-2\,\mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}\right) && \\
\mathcal{F}_{\pi^\pm}(\tilde{\nu},\vartheta_{\pi^+}) &= -\frac{M_\pi^2}{F_\pi^2} & \mathcal{G}_{\pi^\pm}(\tilde{\nu},\vartheta_{\pi^+}) &= \mp\frac{4M_\pi^2}{F_\pi^2}\,\tilde{\nu}\,\mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}} \\
\mathcal{F}_{K^\pm}(\tilde{\nu},\vartheta_{\pi^+}) &= 0 & \mathcal{G}_{K^\pm}(\tilde{\nu},\vartheta_{\pi^+}) &= \mp\frac{2M_K M_\pi}{F_\pi^2}\,\tilde{\nu}\,\mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}} \\
\mathcal{F}_{K^0}(\tilde{\nu},\vartheta_{\pi^+}) &= 0 & \mathcal{G}_{K^0}(\tilde{\nu},\vartheta_{\pi^+}) &= \frac{2M_K M_\pi}{F_\pi^2}\,\tilde{\nu}\,\mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}} \\
\mathcal{F}_{\eta}(\tilde{\nu},\vartheta_{\pi^+}) &= \frac{M_\pi^2}{3F_\pi^2}\left(1+2\mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}\right), &&
\end{aligned}
\tag{3.91}
$$

in the resummed asymptotic formulae. Dropping $\mathcal{O}(\mathrm{e}^{-\bar{\lambda}})$ we find

$$
\begin{aligned}
\delta M_{\pi^0} &= \frac{\xi_\pi}{4}\left[2\,\mathrm{g}_1(\lambda_\pi,\vartheta_{\pi^+})-\mathrm{g}_1(\lambda_\pi)\right] && \\
\delta M_{\pi^\pm} &= \frac{\xi_\pi}{4}\,\mathrm{g}_1(\lambda_\pi) & \Delta\vec{\vartheta}_{\Sigma_{\pi^\pm}} &= \pm\,\xi_\pi\vec{\mathrm{f}}_1(\lambda_\pi,\vartheta_{\pi^+}) \\
\delta M_{K^\pm} &= 0 & \Delta\vec{\vartheta}_{\Sigma_{K^\pm}} &= \pm\,\frac{\xi_\pi}{2}\vec{\mathrm{f}}_1(\lambda_\pi,\vartheta_{\pi^+}) \\
\delta M_{K^0} &= 0 & \Delta\vec{\vartheta}_{\Sigma_{K^0}} &= -\,\frac{\xi_\pi}{2}\vec{\mathrm{f}}_1(\lambda_\pi,\vartheta_{\pi^+}) \\
\delta M_{\eta} &= -\frac{M_\pi^2}{M_\eta^2}\,\frac{\xi_\pi}{12}\,\left[\mathrm{g}_1(\lambda_\pi)+2\,\mathrm{g}_1(\lambda_\pi,\vartheta_{\pi^+})\right]. &&
\end{aligned}
\tag{3.92}
$$

These expressions coincide with the results (2.43, 2.41, 2.76) obtained at NLO in ChPT if contributions of virtual kaons and eta meson are discarded. Note that at tree level the chiral representation of $\mathcal{F}_{K^\pm}(\tilde{\nu},\vartheta_{\pi^+})$, $\mathcal{F}_{K^0}(\tilde{\nu},\vartheta_{\pi^+})$ disappears. This means that the mass corrections of kaons estimated by asymptotic formulae are $\mathcal{O}(\mathrm{e}^{-\bar{\lambda}})$ and hence, negligible.

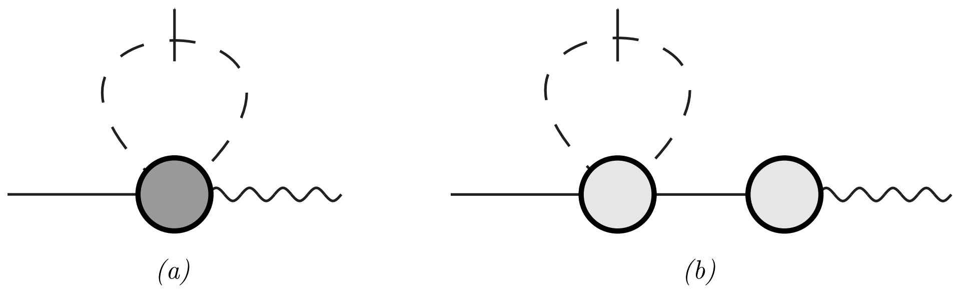


Figure 3.4: Skeleton diagram contributing to asymptotic formulae for decay constants after (a) and before the subtraction of the pole (b). Solid lines stand for a generic pseudoscalar meson P and dashed lines for virtual pions. Wave lines represent the axialvector currents. The spline indicates that the pion propagator is in finite volume and accounts for winding numbers $\vec{n} \in \mathbb{Z}^3$ with $|\vec{n}| = 1$. Blobs in dark (resp. light) gray correspond to vertex functions after (before) the pole subtraction.

3.3 Asymptotic Formulae for Decay Constants

3.3.1 Sketch of the Derivation

The derivation of the asymptotic formulae for decay constants is in large part analogous to that of Section 3.2.2. The main difference is that at the place of the self energies there are now the matrix elements of the axialvector decay. The starting point is to study the asymptotic behaviour of the matrix elements,

$$p_\mu \mathscr{A}^\mu_{ab} = p_\mu \langle 0 | A^\mu_a(0) | \phi_b(p) \rangle \,, \tag{3.93}$$

in finite volume with TBC[4]. One can show that at large volume the dominant contribution to $\mathscr{A}^\mu_{ab}$ is given by the diagram of Fig. 3.4a. The demonstration relies on Abstract Graph Theory and is similar to that of the self energies, see Appendix C. The fact that now one external line represents the axialvector currents does not touch the argumentation at all.

The dominant contribution can then be estimated with the contour integration in the complex plane. One proceeds as in Section 3.2.2 and in case, one expands the vertex functions as in Eq. (3.65). It turns out that the dominant contribution can be expressed as the integral of the amplitude obtained from the diagram of Fig. 3.4a if one breaks up the loop and puts the resulting lines on-shell. This amplitude describes the axialvector decay in infinite volume of the pseudoscalar meson P into two pions and can be determined from

$$p_\mu \langle \pi_c(p_1)\pi_c(p_2) | A^\mu_a(0) | \phi_b(p) \rangle \,. \tag{3.94}$$

Here, $|\pi_c(p_1)\pi_c(p_2)\rangle$ is a two-pion state with a zero isospin and the momenta are in the forward kinematics, i.e. $p^\mu_2 = -p^\mu_1$.

As we know, the matrix elements $\langle \pi_c\pi_c | A^\mu_a | \phi_b \rangle$ has a pole in the forward kinematics. This pole originates from the exchange of an additional virtual pseudoscalar meson P, see

[4]Note that here, we work in Minkowski space where $p^\mu = \left(\begin{smallmatrix} p_0 \\ \vec{p} \end{smallmatrix}\right)$, $k^\mu = \left(\begin{smallmatrix} k_0 \\ \vec{k} \end{smallmatrix}\right)$ and $p_\mu k^\mu = p_0 k_0 - \vec{p}\,\vec{k}$.

Fig. 3.4b. We can understand the presence of the pole if we review the definition of the decay constant [31]. The decay constant is defined as the residue of the two-point function containing the axialvector current and the interpolating field of the pseudoscalar meson, see Eq. (2.48). In finite volume the mass pole as well as the residue are shifted. For charged pions, the mass poles are shifted as $p^2_{\pi^\pm}(L) = (p+\vartheta_{\pi^\pm}+\Delta\vartheta_{\Sigma_{\pi^\pm}})^2 = M^2_{\pi^\pm}(L)$. The residues are shifted by the mass poles and by the two-point functions $P_{\pi^\pm}$. Ignoring the shift of the mass poles corresponds to multiply the two-point functions $P_{\pi^\pm}$ by $[M_\pi^2 - (p+\vartheta_{\pi^\pm})^2]$ instead of $[M^2_{\pi^\pm}(L) - p^2_{\pi^\pm}(L)]$ and then, take the limit $(p+\vartheta_{\pi^\pm})^2 \to M_\pi^2$. This generates the pole term of the Fig. 3.4b.

To explicitly see how the pole term is generated we consider Eq. (2.49) at higher order and multiply the two-point functions with $[M_\pi^2 - (p+\vartheta_{\pi^\pm})^2]$. Up to $\mathcal{O}(\mathrm{e}^{-\bar\lambda})$ we find

$$\begin{aligned}\left[M_\pi^2 - (p+\vartheta_{\pi^\pm})^2\right] P_{\pi^\pm} &= \frac{M_\pi^2 - (p+\vartheta_{\pi^\pm})^2}{M^2_{\pi^\pm}(L) - p^2_{\pi^\pm}(L)} N_{\pi^\pm}\Big[(p+\vartheta_{\pi^\pm})^2 F_{\pi^\pm}(L) \\ &\qquad + 2F_\pi (p+\vartheta_{\pi^\pm})_\mu \Delta\vartheta^\mu_{\mathscr{A}_{\pi^\pm}} + \mathcal{O}(\mathrm{e}^{-\bar\lambda})\Big] \\ &= \left[1 - \frac{\Delta\Sigma_{\pi^\pm}(p+\vartheta_{\pi^\pm})}{M_\pi^2 - (p+\vartheta_{\pi^\pm})^2}\right]^{-1} N_{\pi^\pm}\Big[(p+\vartheta_{\pi^\pm})^2 F_{\pi^\pm}(L) \\ &\qquad + 2F_\pi (p+\vartheta_{\pi^\pm})_\mu \Delta\vartheta^\mu_{\mathscr{A}_{\pi^\pm}} + \mathcal{O}(\mathrm{e}^{-\bar\lambda})\Big].\end{aligned} \tag{3.95}$$

Here, $\Delta\vartheta^\mu_{\mathscr{A}_{\pi^\pm}}$ are the renormalization terms of the matrix elements $\mathscr{A}^\mu_{\pi^\pm} = \langle 0 | A^\mu_{1\mp i2} | \pi^\pm\rangle_L$ at higher order[5]. In the last equality of Eq. (3.95) we use

$$\frac{M_\pi^2 - (p+\vartheta_{\pi^\pm})^2}{M^2_{\pi^\pm}(L) - p^2_{\pi^\pm}(L)} = \left[1 - \frac{\Delta\Sigma_{\pi^\pm}(p+\vartheta_{\pi^\pm})}{M_\pi^2 - (p+\vartheta_{\pi^\pm})^2}\right]^{-1}, \tag{3.96}$$

which follows from

$$\begin{aligned}\left[M^2_{\pi^\pm}(L) - p^2_{\pi^\pm}(L)\right] &= \left[M_\pi^2 + \Delta M^2_{\pi^\pm} - (p+\vartheta_{\pi^\pm}+\Delta\vartheta_{\Sigma_{\pi^\pm}})^2\right] \\ &= \left[M_\pi^2 - (p+\vartheta_{\pi^\pm})^2 - \Delta\Sigma_{\pi^\pm}(p+\vartheta_{\pi^\pm})\right] \\ &= \left[M_\pi^2 - (p+\vartheta_{\pi^\pm})^2\right]\left[1 - \frac{\Delta\Sigma_{\pi^\pm}(p+\vartheta_{\pi^\pm})}{M_\pi^2 - (p+\vartheta_{\pi^\pm})^2}\right].\end{aligned} \tag{3.97}$$

If we expand Eq. (3.95) for asymptotically large volume and retain terms up to $\mathcal{O}(\mathrm{e}^{-\bar\lambda})$,

[5] In Section 2.3.2 we calculated these terms in ChPT at NLO. We have found

$$\Delta\vartheta^\mu_{\mathscr{A}_{\pi^\pm}} = \Delta\vartheta^\mu_{\pi^\pm} + \mathcal{O}(p^5/F_\pi^4),$$

where $\Delta\vartheta^\mu_{\pi^\pm}$ are the extra terms of Eq. (2.49). Note that in ChPT, the renormalization terms $\Delta\vartheta^\mu_{\Sigma_{\pi^\pm}}$, $\Delta\vartheta^\mu_{\mathscr{A}_{\pi^\pm}}$ coincide at NLO and are both given by Eq. (2.31).

we find the poles for $(p+\vartheta_{\pi^\pm})^2 = M_\pi^2$,

$$\left[M_\pi^2 - (p+\vartheta_{\pi^\pm})^2\right] P_{\pi^\pm} \approx F_{\pi^\pm}(L) + 2\,\frac{F_\pi}{M_\pi^2}\,(p+\vartheta_{\pi^\pm})_\mu(\Delta\vartheta_{\mathscr{A}_{\pi^\pm}} - \Delta\vartheta_{\Sigma_{\pi^\pm}})^\mu + F_\pi\,\frac{\Delta\Sigma_{\pi^\pm}(p+\vartheta_{\pi^\pm})}{M_\pi^2 - (p+\vartheta_{\pi^\pm})^2} + \mathcal{O}(\mathrm{e}^{-\bar\lambda}). \quad (3.98)$$

Since we know the formulae of $\Delta\Sigma_{\pi^\pm}$ up to $\mathcal{O}(\mathrm{e}^{-\bar\lambda})$ we can subtract the pole terms from the right-hand side of Eq. (3.98) and obtain asymptotic formulae for $F_{\pi^\pm}(L)$ resp. $\Delta\vartheta^\mu_{\mathscr{A}_{\pi^\pm}}$.

Altogether, the asymptotic formulae for the decay constants read

$$\delta F_{\pi^0} = \frac{1}{(4\pi)^2\lambda_\pi}\,\frac{M_\pi}{F_\pi}\sum_{\substack{\vec n\in\mathbb{Z}^3\\|\vec n|\neq 0}}\int_{\mathbb{R}}\frac{\mathrm{d}y}{|\vec n|}\,\mathrm{e}^{-\lambda_\pi|\vec n|\sqrt{1+y^2}}\,\mathcal{N}_{\pi^0}(iy,\vartheta_{\pi^+}) + \mathcal{O}(\mathrm{e}^{-\bar\lambda}) \quad (3.99a)$$

$$\delta F_{\pi^\pm} = \frac{1}{(4\pi)^2\lambda_\pi}\,\frac{M_\pi}{F_\pi}\sum_{\substack{\vec n\in\mathbb{Z}^3\\|\vec n|\neq 0}}\int_{\mathbb{R}}\frac{\mathrm{d}y}{|\vec n|}\,\mathrm{e}^{-\lambda_\pi|\vec n|\sqrt{1+y^2}} \times\left(1 + y\frac{D_{\pi^\pm}}{M_\pi}\frac{\partial}{\partial y}\right)\mathcal{N}_{\pi^\pm}(iy,\vartheta_{\pi^+}) + \mathcal{O}(\mathrm{e}^{-\bar\lambda}) \quad (3.99b)$$

$$\delta F_{K^\pm} = \frac{1}{(4\pi)^2\,\lambda_K}\,\frac{M_\pi}{F_K}\sum_{\substack{\vec n\in\mathbb{Z}^3\\|\vec n|\neq 0}}\int_{\mathbb{R}}\frac{\mathrm{d}y}{|\vec n|}\,\mathrm{e}^{-\lambda_\pi|\vec n|\sqrt{1+y^2}} \times\left(1 + y\frac{D_{K^\pm}}{M_K}\frac{\partial}{\partial y}\right)\mathcal{N}_{K^\pm}(iy,\vartheta_{\pi^+}) + \mathcal{O}(\mathrm{e}^{-\bar\lambda}) \quad (3.99c)$$

$$\delta F_{K^0} = \frac{1}{(4\pi)^2\,\lambda_K}\,\frac{M_\pi}{F_K}\sum_{\substack{\vec n\in\mathbb{Z}^3\\|\vec n|\neq 0}}\int_{\mathbb{R}}\frac{\mathrm{d}y}{|\vec n|}\,\mathrm{e}^{-\lambda_\pi|\vec n|\sqrt{1+y^2}} \times\left(1 + y\frac{D_{K^0}}{M_K}\frac{\partial}{\partial y}\right)\mathcal{N}_{K^0}(iy,\vartheta_{\pi^+}) + \mathcal{O}(\mathrm{e}^{-\bar\lambda}) \quad (3.99d)$$

$$\delta F_\eta = \frac{1}{(4\pi)^2\,\lambda_\eta}\,\frac{M_\pi}{F_\eta}\sum_{\substack{\vec n\in\mathbb{Z}^3\\|\vec n|\neq 0}}\int_{\mathbb{R}}\frac{\mathrm{d}y}{|\vec n|}\,\mathrm{e}^{-\lambda_\pi|\vec n|\sqrt{1+y^2}}\,\mathcal{N}_\eta(iy,\vartheta_{\pi^+}) + \mathcal{O}(\mathrm{e}^{-\bar\lambda}). \quad (3.99e)$$

Note that we display the resummed version of the formulae for which $\bar\lambda = \bar M L$ with $\bar M = (\sqrt{3}+1)\,M_\pi/\sqrt{2}$. The parameters $D_{\pi^\pm}$, $D_{K^\pm}$, D_{K^0} are given in Eqs. (3.57, 3.83). The amplitudes are all defined in similar way for the various pseudoscalar mesons. For instance, the amplitudes of charged pions are

$$\mathcal{N}_{\pi^\pm}(\tilde{\nu}, \vartheta_{\pi^+}) = -i\Big\{ \bar{A}_{\pi^\pm\pi^0}(0, -4M_\pi\nu) + \left[\bar{A}_{\pi^\pm\pi^+}(0, -4M_\pi\nu) + \bar{A}_{\pi^\pm\pi^-}(0, -4M_\pi\nu)\right] \mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}} \Big\}, \quad (3.100)$$

where $\nu = (u-t)/(4M_\pi)$ and $\tilde{\nu} = \nu/M_\pi = iy$. The functions $\bar{A}_{\pi^\pm\pi^0}(s, t-u)$, $\bar{A}_{\pi^\pm\pi^+}(s, t-u)$, $\bar{A}_{\pi^\pm\pi^-}(s, t-u)$ are the isospin components in infinite volume of the amplitude describing the pion decay into a two-pion state with a zero isospin,

$$\bar{A}_\pi^{I=0}(s, t-u) = \bar{A}_{\pi^\pm\pi^0}(s, t-u) + \bar{A}_{\pi^\pm\pi^+}(s, t-u) + \bar{A}_{\pi^\pm\pi^-}(s, t-u), \quad (3.101)$$

see Ref. [32]. The bar indicates that the pole has been subtracted from the isospin components. In Section 3.3.2 we illustrate how to subtract the pole by means of two examples.

The asymptotic formulae (3.99) generalize the formulae for pseudoscalar mesons presented in Eq. (23) of Ref. [32]. They estimate the corrections of the decay constants in finite volume with TBC. The dependence on twist is twofold. On one hand the formulae depend on the twisting angle of the virtual positive pion through the phase factor $\exp(iL\vec{n}\vec{\vartheta}_{\pi^+})$ in the amplitudes. On the other hand the formulae depend on the external twisting angles through the parameters $D_{\pi^\pm}, D_{K^\pm}, D_{K^0}$. If we set all twisting angles to zero we recover the formulae valid for PBC and presented in Ref. [32]. Note that the formulae for charged pions and kaons are valid for small external twisting angles as they result from expansions like Eq. (3.65). On the contrary, the formulae for the neutral pion and the eta meson are valid for arbitrary twisting angles.

In Section 3.2.3 we briefly discuss how to derive asymptotic formulae for the renormalization terms of self energies. In an analogous way we can derive asymptotic formulae for the renormalization terms of the matrix elements considered here. We obtain

$$\Delta\vec{\vartheta}_{\mathscr{A}_{\pi^\pm}} = -\frac{1}{2\,(4\pi)^2}\frac{M_\pi^2}{F_\pi}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\frac{\vec{n}}{|\vec{n}|}\int_{\mathbb{R}} \mathrm{d}y\ \mathrm{e}^{-\lambda_\pi|\vec{n}|\sqrt{1+y^2}}\ y\ \mathcal{H}_{\pi^\pm}(iy, \vartheta_{\pi^+}) + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}}) \quad (3.102a)$$

$$\Delta\vec{\vartheta}_{\mathscr{A}_{K^\pm}} = -\frac{1}{2\,(4\pi)^2}\frac{M_\pi^2}{F_K}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\frac{\vec{n}}{|\vec{n}|}\int_{\mathbb{R}} \mathrm{d}y\ \mathrm{e}^{-\lambda_\pi|\vec{n}|\sqrt{1+y^2}}\ y\ \mathcal{H}_{K^\pm}(iy, \vartheta_{\pi^+}) + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}}) \quad (3.102b)$$

$$\Delta\vec{\vartheta}_{\mathscr{A}_{K^0}} = -\frac{1}{2\,(4\pi)^2}\frac{M_\pi^2}{F_K}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\frac{\vec{n}}{|\vec{n}|}\int_{\mathbb{R}} \mathrm{d}y\ \mathrm{e}^{-\lambda_\pi|\vec{n}|\sqrt{1+y^2}}\ y\ \mathcal{H}_{K^0}(iy, \vartheta_{\pi^+}) + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}}). \quad (3.102c)$$

Here, $\Delta\vartheta^\mu_{\mathscr{A}_{K^\pm}}$ (resp. $\Delta\vartheta^\mu_{\mathscr{A}_{K^0}}$) represent the renormalization terms of $\mathscr{A}^\mu_{K^\pm} = \langle 0|\, A^\mu_{4\mp i5}\,|K^\pm\rangle_L$ (resp. $\mathscr{A}^\mu_{K^0} = \langle 0|\, A^\mu_{6-i7}\,|K^0\rangle_L$). These formulae are valid for small external twisting angles. The amplitudes are given by the difference of the isospin components. For instance,

$$\mathcal{H}_{\pi^\pm}(\tilde{\nu}, \vartheta_{\pi^+}) = -i\left[\bar{A}_{\pi^\pm\pi^+}(0, -4M_\pi\nu) - \bar{A}_{\pi^\pm\pi^-}(0, -4M_\pi\nu)\right] \mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}. \quad (3.103)$$

Note that for $\vartheta^\mu_{\pi^+} = 0$ the sums in Eq. (3.102) are odd in $\vec{n}$ and hence, disappear. This is in accordance with the expectation that renormalization terms are not present in finite volume with PBC.

3.3.2 Pole Subtraction

In ChPT the matrix elements (3.94) have been calculated for charged pions in Ref. [47] and charged kaons in Ref. [48]. We use these results to illustrate the pole subtraction leading to the amplitudes entering the asymptotic formulae (3.99, 3.102).

The amplitudes of charged pions can be determined from the matrix elements of the tau decay $\tau \longrightarrow 3\pi\,\nu_\tau$, see Ref. [47]. We define,

$$(A_{\pi^-\pi^0})^\mu = \left\langle \pi^0(p_1)\pi^0(p_2)\pi^-(p_3)\right| A^\mu_{1-i2}(0)\,|0\rangle \tag{3.104a}$$

$$(A_{\pi^-\pi^-})^\mu = \left\langle \pi^-(p_1)\pi^+(p_2)\pi^-(p_3)\right| A^\mu_{1-i2}(0)\,|0\rangle\,. \tag{3.104b}$$

According to [47] these matrix elements can be decomposed[6]as

$$(A_{\pi^-\pi^0})^\mu = F_{123}\,p_3^\mu + G_{123}\,(p_1+p_2)^\mu + H_{123}\,(p_1-p_2)^\mu \tag{3.105a}$$

$$(A_{\pi^-\pi^-})^\mu = F^{[-]}_{123}\,p_3^\mu + G^{[-]}_{123}(p_1+p_2)^\mu + H^{[-]}_{123}(p_1-p_2)^\mu. \tag{3.105b}$$

The factors $F_{123} = F(s_1,s_2,s_3)$, $G_{123} = G(s_1,s_2,s_3)$, $H_{123} = H(s_1,s_2,s_3)$ are scalar functions of the variables

$$\begin{aligned} s_1 &= (p_2+p_3)^2 \\ s_2 &= (p_1+p_3)^2 \\ s_3 &= (p_1+p_2)^2, \end{aligned} \tag{3.106}$$

and satisfy the properties,

$$\begin{aligned} F_{213} &= F_{123} \\ G_{213} &= G_{123} \\ H_{213} &= -H_{123}. \end{aligned} \tag{3.107}$$

They are related to $F^{[-]}_{123} = F^{[-]}(s_1,s_2,s_3)$, $G^{[-]}_{123} = G^{[-]}(s_1,s_2,s_3)$, $H^{[-]}_{123} = H^{[-]}(s_1,s_2,s_3)$ by virtue of

$$\begin{aligned} F^{[-]}_{123} &= F_{123} + G_{231} - H_{231} \\ G^{[-]}_{123} &= G_{123} + \frac{1}{2}\left[F_{231} + G_{231} + H_{231}\right] \\ H^{[-]}_{123} &= H_{123} + \frac{1}{2}\left[F_{231} - G_{231} - H_{231}\right]. \end{aligned} \tag{3.108}$$

The factors $F_{123}, G_{123}, H_{123}$ are calculated up to NLO in Section 4.2 of Ref. [47].

To subtract the pole from the matrix elements we must expand (3.105) in the neighbourhood of $Q^2 = (p_1+p_2+p_3)^2 = M_\pi^2$. The pole appears in the factors F_{123}, G_{123} resp. $F^{[-]}_{123}, G^{[-]}_{123}$ and can be expressed in terms of the $\pi\pi$-scattering amplitude, see Ref. [47]. We obtain

$$\begin{aligned} (\bar{A}_{\pi^-\pi^0})^\mu &= (A_{\pi^-\pi^0})^\mu - iF_\pi Q^\mu \frac{T_{\pi^-\pi^0}(s_3, s_1-s_2)}{M_\pi^2 - Q^2} \\ (\bar{A}_{\pi^-\pi^-})^\mu &= (A_{\pi^-\pi^-})^\mu - iF_\pi Q^\mu \frac{T_{\pi^-\pi^-}(s_3, s_1-s_2)}{M_\pi^2 - Q^2}, \end{aligned} \tag{3.109}$$

[6]The factors $F_{123}, G_{123}, H_{123}$ are $1/\sqrt{2}$ times smaller than those of Ref. [47].

where $T_{\pi^-\pi^0}(s_3, s_1-s_2)$ resp. $T_{\pi^-\pi^-}(s_3, s_1-s_2)$ are isospin components of the $\pi\pi$-scattering amplitude in the s_3-channel, given in Eq. (4.4). The bar indicates that the pole has been subtracted from the matrix element.

The amplitudes entering the asymptotic formulae (3.99b, 3.102a) can be obtained through the contraction with p_3^μ/M_π and setting the momenta $p_2^\mu = -p_1^\mu$ resp. $p_3^\mu = \left(\begin{smallmatrix} M_\pi \\ \vec{0} \end{smallmatrix}\right)$. The amplitude of the negative pion reads

$$\begin{aligned}\mathcal{N}_{\pi^-}(\tilde{\nu}, \vartheta_{\pi^+}) = -i\Big\{&\bar{A}_{\pi^-\pi^0}(0, -4M_\pi\nu) \\ &+ \left[\bar{A}_{\pi^-\pi^-}(0, -4M_\pi\nu) + \bar{A}_{\pi^-\pi^+}(0, -4M_\pi\nu)\right] \mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}\Big\}\end{aligned} \tag{3.110a}$$

$$\mathcal{H}_{\pi^-}(\tilde{\nu}, \vartheta_{\pi^+}) = -i\left[\bar{A}_{\pi^-\pi^+}(0, -4M_\pi\nu) - \bar{A}_{\pi^-\pi^-}(0, -4M_\pi\nu)\right] \mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}, \tag{3.110b}$$

where $\nu = (s_2-s_1)/(4M_\pi)$ and $\tilde{\nu} = \nu/M_\pi = iy$. The isospin components $\bar{A}_{\pi^-\pi^0}(s_3, s_1-s_2)$, $\bar{A}_{\pi^-\pi^-}(s_3, s_1-s_2)$, $\bar{A}_{\pi^-\pi^+}(s_3, s_1-s_2)$ are given by the contraction of the matrix elements with p_3^μ/M_π,

$$\begin{aligned}\bar{A}_{\pi^-\pi^0}(s_3, s_1-s_2) &= \frac{p_3^\mu}{M_\pi}\left(\bar{A}_{\pi^-\pi^0}\right)_\mu \\ \bar{A}_{\pi^-\pi^-}(s_3, s_1-s_2) &= \frac{p_3^\mu}{M_\pi}\left(\bar{A}_{\pi^-\pi^-}\right)_\mu \\ \bar{A}_{\pi^-\pi^+}(s_3, s_1-s_2) &= \frac{p_3^\mu}{M_\pi}\left(\bar{A}_{\pi^-\pi^+}\right)_\mu .\end{aligned} \tag{3.111}$$

Here, $\bar{A}_{\pi^-\pi^+}(s_3, s_1-s_2)$ is defined by exchanging $p_1^\mu \leftrightarrow p_2^\mu$ in the matrix element (3.104b). The sum of the isospin components amounts to the amplitude describing the decay in the s_3-channel of the pion into two a (2π)-state with a zero isospin,

$$\bar{A}_\pi^{I=0}(s_3, s_1-s_2) = \bar{A}_{\pi^-\pi^0}(s_3, s_1-s_2) + \bar{A}_{\pi^-\pi^+}(s_3, s_1-s_2) + \bar{A}_{\pi^-\pi^-}(s_3, s_1-s_2), \tag{3.112}$$

see Ref. [32]. Note that isospin symmetry relates the amplitudes of the negative pion to those of the positive pion via

$$\mathcal{N}_{\pi^+}(\tilde{\nu}, \vartheta_{\pi^+}) = \mathcal{N}_{\pi^-}(\tilde{\nu}, \vartheta_{\pi^+}) \tag{3.113a}$$

$$\mathcal{H}_{\pi^+}(\tilde{\nu}, \vartheta_{\pi^+}) = -\mathcal{H}_{\pi^-}(\tilde{\nu}, \vartheta_{\pi^+}). \tag{3.113b}$$

We can now apply the asymptotic formulae at tree level. Inserting the chiral representation,

$$\begin{aligned}\mathcal{N}_{\pi^\pm}(\tilde{\nu}, \vartheta_{\pi^+}) &= -\frac{M_\pi}{F_\pi}\left(1 + \mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}\right) \\ \mathcal{H}_{\pi^\pm}(\tilde{\nu}, \vartheta_{\pi^+}) &= \mp\frac{4M_\pi}{F_\pi}\,\tilde{\nu}\,\mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}},\end{aligned} \tag{3.114}$$

and dropping $\mathcal{O}(\mathrm{e}^{-\bar{\lambda}})$ we obtain

$$\begin{aligned}\delta F_{\pi^\pm} &= -\frac{\xi_\pi}{2}\left[\mathrm{g}_1(\lambda_\pi) + \mathrm{g}_1(\lambda_\pi, \vartheta_{\pi^+})\right] \\ \Delta\vec{\vartheta}_{\mathscr{A}_{\pi^\pm}} &= \pm\,\xi_\pi\vec{\mathrm{f}}_1(\lambda_\pi, \vartheta_{\pi^+}).\end{aligned} \tag{3.115}$$

These expressions coincide with Eqs. (2.75b, 2.76).

The amplitudes of the charged kaons can be determined from the matrix elements of the $K_{\ell 4}$ decay, see Ref. [48]. We define,

$$(A_{K^+\pi^0})^\mu = \left\langle \pi^0(p_1)\pi^0(p_2)\right| A^\mu_{4-i5}(0) \left|K^+(p_3)\right\rangle \tag{3.116a}$$
$$(A_{K^+\pi^+})^\mu = \left\langle \pi^+(p_1)\pi^-(p_2)\right| A^\mu_{4-i5}(0) \left|K^+(p_3)\right\rangle . \tag{3.116b}$$

According to [48] these matrix elements can be decomposed[7] as

$$(A_{K^+\pi^0})^\mu = \frac{-i}{M_K}\left[F^+_{stu}\,(p_1+p_2)^\mu + G^-_{stu}\,(p_1-p_2)^\mu + R^+_{stu}\,\tilde{Q}^\mu\right] \tag{3.117a}$$
$$(A_{K^+\pi^+})^\mu = \frac{-i}{M_K}\left[F_{stu}\,(p_1+p_2)^\mu + G_{stu}\,(p_1-p_2)^\mu + R_{stu}\,\tilde{Q}^\mu\right], \tag{3.117b}$$

where $\tilde{Q}^\mu = (p_3 - p_1 - p_2)^\mu$. The factors $F^+_{stu} = F^+(s,t,u)$, $G^-_{stu} = G^-(s,t,u)$, $R^+_{stu} = R^+(s,t,u)$ are scalar functions of the Mandelstam variables (3.14) and satisfy the properties,

$$\begin{aligned} F^+_{sut} &= F^+_{stu} \\ G^-_{sut} &= -G^-_{stu} \\ R^+_{sut} &= R^+_{stu}. \end{aligned} \tag{3.118}$$

They are related to $F_{stu} = F(s,t,u)$, $G_{stu} = G(s,t,u)$, $R_{stu} = R(s,t,u)$ by virtue of

$$\begin{aligned} F^+_{stu} &= \frac{1}{2}\left[F_{stu} + F_{sut}\right] \\ G^-_{stu} &= \frac{1}{2}\left[G_{stu} - G_{sut}\right] \\ R^+_{stu} &= \frac{1}{2}\left[R_{stu} + R_{sut}\right]. \end{aligned} \tag{3.119}$$

The factors $F_{stu}, G_{stu}, R_{stu}$ are calculated up to NLO in Section 3.2 of Ref. [48].

To subtract the pole from the matrix elements we must expand (3.117) in the neighbourhood of $\tilde{Q}^2 = M_K^2$. The pole appears in the factors R^+_{stu} resp. R_{stu} and can be expressed in terms of the $K\pi$-scattering amplitude, see [48]. We obtain

$$\begin{aligned} (\bar{A}_{K^+\pi^0})^\mu &= (A_{K^+\pi^0})^\mu - iF_K\tilde{Q}^\mu\frac{T_{K^+\pi^0}(s,t-u)}{M_K^2-\tilde{Q}^2} \\ (\bar{A}_{K^+\pi^+})^\mu &= (A_{K^+\pi^+})^\mu - iF_K\tilde{Q}^\mu\frac{T_{K^+\pi^+}(s,t-u)}{M_K^2-\tilde{Q}^2}, \end{aligned} \tag{3.120}$$

where $T_{K^+\pi^0}(s,t-u)$, $T_{K^+\pi^+}(s,t-u)$ are isospin components of the $K\pi$-scattering in the s-channel, see Eq. (4.23), The amplitudes entering the asymptotic formulae (3.99c,

[7] The factors $F_{stu}, G_{stu}, R_{stu}$ are $1/\sqrt{2}$ times smaller than those of Ref. [48].

3.102b) can be obtained through the contraction with p_3^μ/M_K and by setting $p_2^\mu = -p_1^\mu$ and $p_3^\mu = \left(\begin{smallmatrix} M_K \\ \vec{0} \end{smallmatrix}\right)$. For the positive kaon we have

$$\begin{aligned}\mathcal{N}_{K^+}(\tilde{\nu}, \vartheta_{\pi^+}) = -i\Big\{&\bar{A}_{K^+\pi^0}(0, -4M_K\nu) \\ &+ \left[\bar{A}_{K^+\pi^+}(0, -4M_K\nu) + \bar{A}_{K^+\pi^-}(0, -4M_K\nu)\right] \mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}\Big\}\end{aligned} \tag{3.121a}$$

$$\mathcal{H}_{K^+}(\tilde{\nu}, \vartheta_{\pi^+}) = -i\left[\bar{A}_{K^+\pi^+}(0, -4M_K\nu) - \bar{A}_{K^+\pi^-}(0, -4M_K\nu)\right] \mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}, \tag{3.121b}$$

where $\nu = (u-t)/(4M_K)$ and $\tilde{\nu} = \nu/M_\pi = iy$. The isospin components $\bar{A}_{K^+\pi^0}(s, t-u)$, $\bar{A}_{K^+\pi^+}(s, t-u)$, $\bar{A}_{K^+\pi^-}(s, t-u)$ are given by the contraction of the matrix elements with p^μ/M_K,

$$\begin{aligned}\bar{A}_{K^+\pi^0}(s, t-u) &= \frac{p^\mu}{M_K}(\bar{A}_{K^+\pi^0})_\mu \\ \bar{A}_{K^+\pi^+}(s, t-u) &= \frac{p^\mu}{M_K}(\bar{A}_{K^+\pi^+})_\mu \\ \bar{A}_{K^+\pi^-}(s, t-u) &= \frac{p^\mu}{M_K}(\bar{A}_{K^+\pi^-})_\mu .\end{aligned} \tag{3.122}$$

Here, $\bar{A}_{K^+\pi^-}(s, t-u)$ is defined by exchanging $p_1^\mu \leftrightarrow p_2^\mu$ in the matrix element (3.116b). Note that the isospin symmetry relates the amplitudes of the positive kaon to those of the negative kaon via

$$\mathcal{N}_{K^-}(\tilde{\nu}, \vartheta_{\pi^+}) = \mathcal{N}_{K^+}(\tilde{\nu}, \vartheta_{\pi^+}) \tag{3.123a}$$
$$\mathcal{H}_{K^-}(\tilde{\nu}, \vartheta_{\pi^+}) = -\mathcal{H}_{K^+}(\tilde{\nu}, \vartheta_{\pi^+}). \tag{3.123b}$$

Inserting the chiral representation at tree level,

$$\begin{aligned}\mathcal{N}_{K^\pm}(\tilde{\nu}, \vartheta_{\pi^+}) &= -\frac{M_K}{4F_\pi}\left(1 + 2\mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}\right) \\ \mathcal{H}_{K^\pm}(\tilde{\nu}, \vartheta_{\pi^+}) &= \mp\frac{2M_\pi}{F_\pi}\,\tilde{\nu}\,\mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}},\end{aligned} \tag{3.124}$$

and dropping $\mathcal{O}(\mathrm{e}^{-\bar{\lambda}})$ one obtains

$$\begin{aligned}\delta F_{K^\pm} &= -\frac{\xi_\pi}{8}\left[\mathrm{g}_1(\lambda_\pi) + 2\,\mathrm{g}_1(\lambda_\pi, \vartheta_{\pi^+})\right] \\ \Delta\vec{\vartheta}_{\mathscr{A}_{K^\pm}} &= \pm\frac{\xi_\pi}{2}\vec{\mathrm{f}}_1(\lambda_\pi, \vartheta_{\pi^+}).\end{aligned} \tag{3.125}$$

These expressions coincide with the results (2.54c, 2.41a) if the contributions of virtual kaons and eta meson are discarded.

3.4 Asymptotic Formulae for Pseudoscalar Coupling Constants

3.4.1 Sketch of the Derivation

The derivation of the asymptotic formulae for pseudoscalar coupling constants is similar to that for decay constants, see Section 3.3.1. In this case, the starting point is to consider the matrix elements of the pseudoscalar decay,

$$\mathscr{G}_{ab} = \langle 0|\, P_a(0)\, |\phi_b(p)\rangle\,, \tag{3.126}$$

in finite volume with TBC. One can show that at large volume the dominant contribution to $\mathscr{G}_{ab}$ is given by a diagram similar to Fig. 3.4a where the wave line represent the pseudoscalar densities. The dominant contribution can be estimated with the contour integration as in Section 3.2.2. It turns out that one can express the dominant contribution as the integral of the amplitude describing the pseudoscalar decay into two pions. This amplitude can be determined from the matrix elements,

$$\langle \pi_c(p_1)\pi_c(p_2)|\, P_a(0)\, |\phi_b(p_3)\rangle\,, \tag{3.127}$$

in the forward kinematics. As we know, the matrix elements $\langle \pi_c\pi_c|\, P_a\, |\phi_b\rangle$ have a pole in the forward kinematics. The pole does not contribute to the corrections of the pseudoscalar coupling constant and must be subtracted by means of a prescription similar to the one of Section 3.3.2. The amplitude resulting from the prescription is analytic up to physical cuts starting at $\nu = \pm M_\pi$, see Fig. 3.1.

Altogether, we find the following asymptotic formulae for the pseudoscalar coupling constants,

$$\delta G_{\pi^0} = \frac{1}{(4\pi)^2\lambda_\pi}\,\frac{M_\pi^2}{G_\pi} \sum_{\substack{\vec{n}\in\mathbb{Z}^3\\ |\vec{n}|\neq 0}} \int_{\mathbb{R}} \frac{\mathrm{d}y}{|\vec{n}|}\, \mathrm{e}^{-\lambda_\pi|\vec{n}|\sqrt{1+y^2}}\, \mathcal{C}_{\pi^0}(iy,\vartheta_{\pi^+}) + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}}) \tag{3.128a}$$

$$\delta G_{\pi^\pm} = \frac{1}{(4\pi)^2\lambda_\pi}\,\frac{M_\pi^2}{G_\pi} \sum_{\substack{\vec{n}\in\mathbb{Z}^3\\ |\vec{n}|\neq 0}} \int_{\mathbb{R}} \frac{\mathrm{d}y}{|\vec{n}|}\, \mathrm{e}^{-\lambda_\pi|\vec{n}|\sqrt{1+y^2}} \times \left(1 + y\frac{D_{\pi^\pm}}{M_\pi}\frac{\partial}{\partial y}\right) \mathcal{C}_{\pi^\pm}(iy,\vartheta_{\pi^+}) + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}}) \tag{3.128b}$$

$$\delta G_{K^\pm} = \frac{1}{(4\pi)^2 \lambda_K} \frac{M_\pi M_K}{G_K} \sum_{\substack{\vec{n}\in\mathbb{Z}^3 \\ |\vec{n}|\neq 0}} \int_{\mathbb{R}} \frac{\mathrm{d}y}{|\vec{n}|} \, \mathrm{e}^{-\lambda_\pi |\vec{n}|\sqrt{1+y^2}} \times \left(1 + y \frac{D_{K^\pm}}{M_K} \frac{\partial}{\partial y}\right) \mathcal{C}_{K^\pm}(iy, \vartheta_{\pi^+}) + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}}) \quad (3.128\text{c})$$

$$\delta G_{K^0} = \frac{1}{(4\pi)^2 \lambda_K} \frac{M_\pi M_K}{G_K} \sum_{\substack{\vec{n}\in\mathbb{Z}^3 \\ |\vec{n}|\neq 0}} \int_{\mathbb{R}} \frac{\mathrm{d}y}{|\vec{n}|} \, \mathrm{e}^{-\lambda_\pi |\vec{n}|\sqrt{1+y^2}} \times \left(1 + y \frac{D_{K^0}}{M_K} \frac{\partial}{\partial y}\right) \mathcal{C}_{K^0}(iy, \vartheta_{\pi^+}) + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}}) \quad (3.128\text{d})$$

$$\delta G_{\eta} = \frac{1}{(4\pi)^2 \lambda_\eta} \frac{M_\pi M_\eta}{G_\eta} \sum_{\substack{\vec{n}\in\mathbb{Z}^3 \\ |\vec{n}|\neq 0}} \int_{\mathbb{R}} \frac{\mathrm{d}y}{|\vec{n}|} \, \mathrm{e}^{-\lambda_\pi |\vec{n}|\sqrt{1+y^2}} \, \mathcal{C}_{\eta}(iy, \vartheta_{\pi^+}) + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}}). \quad (3.128\text{e})$$

Note that we display the resummed version of the formulae. The parameters $D_{\pi^\pm}$, $D_{K^\pm}$, D_{K^0} are given in Eqs. (3.57, 3.83). The amplitudes are all defined in similar way for the various pseudoscalar mesons. For instance, the amplitudes of charged pions read

$$\mathcal{C}_{\pi^\pm}(\tilde{\nu}, \vartheta_{\pi^+}) = \bar{C}_{\pi^\pm\pi^0}(0, -4M_\pi\nu) + \left[\bar{C}_{\pi^\pm\pi^+}(0, -4M_\pi\nu) + \bar{C}_{\pi^\pm\pi^-}(0, -4M_\pi\nu)\right] \mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}, \quad (3.129)$$

where $\bar{C}_{\pi^\pm\pi^0}(s, t-u)$, $\bar{C}_{\pi^\pm\pi^+}(s, t-u)$, $\bar{C}_{\pi^\pm\pi^-}(s, t-u)$ can be determined from the matrix elements,

$$\begin{aligned} C_{\pi^\pm\pi^0} &= \left\langle \pi^0(p_1)\pi^0(p_2) \right| P_{1\mp i2}(0) \left| \pi^\pm(p_3) \right\rangle \\ C_{\pi^\pm\pi^+} &= \left\langle \pi^+(p_1)\pi^-(p_2) \right| P_{1\mp i2}(0) \left| \pi^\pm(p_3) \right\rangle \\ C_{\pi^\pm\pi^-} &= \left\langle \pi^-(p_1)\pi^+(p_2) \right| P_{1\mp i2}(0) \left| \pi^\pm(p_3) \right\rangle , \end{aligned} \quad (3.130)$$

after the pole subtraction,

$$\begin{aligned} \bar{C}_{\pi^\pm\pi^0}(s, t-u) &= C_{\pi^\pm\pi^0} - G_\pi \frac{T_{\pi^\pm\pi^0}(s, t-u)}{M_\pi^2 - \tilde{Q}^2} \\ \bar{C}_{\pi^\pm\pi^+}(s, t-u) &= C_{\pi^\pm\pi^+} - G_\pi \frac{T_{\pi^\pm\pi^+}(s, t-u)}{M_\pi^2 - \tilde{Q}^2} \\ \bar{C}_{\pi^\pm\pi^-}(s, t-u) &= C_{\pi^\pm\pi^-} - G_\pi \frac{T_{\pi^\pm\pi^-}(s, t-u)}{M_\pi^2 - \tilde{Q}^2}. \end{aligned} \quad (3.131)$$

Here, $\tilde{Q}^\mu = (p_3 - p_1 - p_2)^\mu$ and $T_{\pi^\pm\pi^0}(s, t-u)$, $T_{\pi^\pm\pi^+}(s, t-u)$, $T_{\pi^\pm\pi^-}(s, t-u)$ are the isospin components (3.81) in the s-channel.

The formulae (3.128) are similar to the asymptotic formulae derived before. Their dependence on the twist is twofold: they depend on the twisting angle of the virtual positive pion through the phase factor $\exp(iL\vec{n}\vec{\vartheta}_{\pi^+})$ and on the external twisting angles through the parameters $D_{\pi^\pm}$, $D_{K^\pm}$, D_{K^0}. If all twisting angles are set to zero the formulae for pions reduce to the formula valid for PBC and presented in Ref. [31]. We stress that the formulae for charged pions and kaons are valid for small external twisting angles because result from expansions like Eq. (3.65). On the contrary, the formulae for the neutral pion and the eta meson are valid for arbitrary twisting angles.

Analogously, we find asymptotic formulae for the renormalization terms. The resummed version reads

$$\Delta\vec{\vartheta}_{\mathscr{G}_{\pi^\pm}} = -\frac{1}{2\,(4\pi)^2}\frac{M_\pi}{G_\pi}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\frac{\vec{n}}{|\vec{n}|}\int_{\mathbb{R}} \mathrm{d}y\ \mathrm{e}^{-\lambda_\pi|\vec{n}|\sqrt{1+y^2}}\ y\ \mathcal{K}_{\pi^\pm}(iy,\vartheta_{\pi^+}) + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}}) \tag{3.132a}$$

$$\Delta\vec{\vartheta}_{\mathscr{G}_{K^\pm}} = -\frac{1}{2\,(4\pi)^2}\frac{M_\pi^2}{G_K M_K}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\frac{\vec{n}}{|\vec{n}|}\int_{\mathbb{R}} \mathrm{d}y\ \mathrm{e}^{-\lambda_\pi|\vec{n}|\sqrt{1+y^2}}\ y\ \mathcal{K}_{K^\pm}(iy,\vartheta_{\pi^+}) + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}}) \tag{3.132b}$$

$$\Delta\vec{\vartheta}_{\mathscr{G}_{K^0}} = -\frac{1}{2\,(4\pi)^2}\frac{M_\pi^2}{G_K M_K}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\frac{\vec{n}}{|\vec{n}|}\int_{\mathbb{R}} \mathrm{d}y\ \mathrm{e}^{-\lambda_\pi|\vec{n}|\sqrt{1+y^2}}\ y\ \mathcal{K}_{K^0}(iy,\vartheta_{\pi^+}) + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}}). \tag{3.132c}$$

Here, $\Delta\vartheta^\mu_{\mathscr{G}_{\pi^\pm}}$, $\Delta\vartheta^\mu_{\mathscr{G}_{K^\pm}}$, $\Delta\vartheta^\mu_{\mathscr{G}_{K^0}}$ represent the renormalization terms of the matrix elements,

$$\begin{aligned}\mathscr{G}_{\pi^\pm} &= \langle 0|\, P_{1\mp i2}(0)\,\big|\pi^\pm(p+\vartheta_{\pi^\pm})\big\rangle_L\\ \mathscr{G}_{K^\pm} &= \langle 0|\, P_{4\mp i5}(0)\,\big|K^\pm(p+\vartheta_{K^\pm})\big\rangle_L\\ \mathscr{G}_{K^0} &= \langle 0|\, P_{6-i7}(0)\,\big|K^0(p+\vartheta_{K^0})\big\rangle_L\,.\end{aligned} \tag{3.133}$$

The formulae (3.132) are valid for small external twisting angles. The amplitudes are given by the difference of the isospin components, e.g.

$$\mathcal{K}_{\pi^\pm}(\tilde{\nu},\vartheta_{\pi^+}) = \left[\bar{C}_{\pi^\pm\pi^+}(0,-4M_\pi\nu) - \bar{C}_{\pi^\pm\pi^-}(0,-4M_\pi\nu)\right]\mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}\,. \tag{3.134}$$

Note that for $\vartheta^\mu_{\pi^+} = 0$ the sums in Eq. (3.132) are odd in $\vec{n}$ and hence, disappear. This is in accordance with the expectation that renormalization terms are not present in finite volume with PBC.

Among the amplitudes entering the asymptotic formulae of Eqs. (3.128, 3.132) only those of pions are known in ChPT. They can be determined from the off-shell amplitude of the point function containing four pseudoscalar densities, see Eq. (16.4) of Ref. [10]. In this case, three pseudoscalar densities serve as interpolating fields for pions and the fourth is left unchanged. The pole affecting the off-shell amplitude can be subtracted by means of the prescription (3.131). The results are the chiral representation for $\mathcal{C}_{\pi^0}(\tilde{\nu}, \vartheta_{\pi^+})$, $\mathcal{C}_{\pi^\pm}(\tilde{\nu}, \vartheta_{\pi^+})$, $\mathcal{K}_{\pi^\pm}(\tilde{\nu}, \vartheta_{\pi^+})$ at one loop. As check we take the tree-level,

$$\mathcal{C}_{\pi^0}(\tilde{\nu}, \vartheta_{\pi^+}) = -\frac{G_\pi}{F_\pi^2} \qquad \mathcal{C}_{\pi^\pm}(\tilde{\nu}, \vartheta_{\pi^+}) = -\frac{G_\pi}{F_\pi^2}\,\tilde{\nu}\,\mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}} \qquad \mathcal{K}_{\pi^\pm}(\tilde{\nu}, \vartheta_{\pi^+}) = 0, \tag{3.135}$$

and feed Eqs. (3.128, 3.132). Dropping $\mathcal{O}(\mathrm{e}^{-\bar{\lambda}})$ we find

$$\delta G_{\pi^0} = -\frac{\xi_\pi}{2}\,\mathrm{g}_1(\lambda_\pi) \qquad \delta G_{\pi^\pm} = -\frac{\xi_\pi}{2}\,\mathrm{g}_1(\lambda_\pi, \vartheta_{\pi^+}) \qquad \Delta\vec{\vartheta}_{\mathscr{G}_{\pi^\pm}} = \vec{0}. \tag{3.136}$$

These expressions coincide with the results (2.75c) obtained in 2-light-flavor ChPT at NLO. Note that $\mathcal{K}_{\pi^\pm}(\tilde{\nu}, \vartheta_{\pi^+}) = 0$ at this order. This is in accordance with the results of Section 2.3.3, namely that no renormalization terms $\Delta\vartheta^\mu_{\mathscr{G}_{\pi^\pm}}$ appear at NLO. Such terms will appear from NNLO onwards.

3.4.2 Chiral Ward Identities

In Ref. [31] Colangelo and Häfeli pointed out that the asymptotic formulae for masses, decay constants and pseudoscalar coupling constants are related by means of chiral Ward identities. They showed that

$$\delta G_\pi = 2\,\delta M_\pi + \delta F_\pi + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}}), \tag{3.137}$$

where δM_π, δF_π, δG_π are given in terms of Eqs. (3.1, 3.2). The relation holds only if the amplitudes entering the asymptotic formulae satisfy the condition[8]

$$\frac{\hat{m}}{M_\pi}\,\mathcal{C}_\pi(\tilde{\nu}) = \mathcal{N}_\pi(\tilde{\nu}) - \frac{F_\pi}{M_\pi}\,\mathcal{F}_\pi(\tilde{\nu}). \tag{3.138}$$

In the following we demonstrate that the relation (3.137) can be generalized to finite volume with TBC and in turn, that the amplitudes satisfy conditions similar to Eq. (3.138).

We start from the relevant chiral Ward identities needed to obtain the above relation. We introduce the twist as in Section 2.2 through the constant vector field v^μ_ϑ. In Section 2.3.3 we have seen that the twist modifies chiral Ward identities in the measure that each momentum is shifted by the corresponding twisting angle. In momentum space, the

[8] In Ref. [31] the condition given in Eq. (15) has a typo. As noted by Häfeli in his PhD thesis [133] the prefactor $\hat{m}/M_\pi$ was originally forgotten.

relevant chiral Ward identities we need, are

$$-i\tilde{Q}_\mu \langle\pi_c(p_1)\pi_c(p_2)|\, A_3^\mu(0)\, |\pi^0(p_3)\rangle = \hat{m}\, \langle\pi_c(p_1)\pi_c(p_2)|\, P_3(0)\, |\pi^0(p_3)\rangle \tag{3.139a}$$

$$\begin{aligned}-i(\tilde{Q}+\vartheta_{\pi^\pm})_\mu \langle\pi_c(p_1)\pi_c(p_2)|\, A^\mu_{1\mp i2}(0)\, |\pi^\pm(p_3+\vartheta_{\pi^\pm})\rangle &= \\ = \hat{m}\, \langle\pi_c(p_1)\pi_c(p_2)|\, P_{1\mp i2}(0)\, |\pi^\pm(p_3+\vartheta_{\pi^\pm})\rangle&\end{aligned} \tag{3.139b}$$

$$\begin{aligned}-i(\tilde{Q}+\vartheta_{K^\pm})_\mu \langle\pi_c(p_1)\pi_c(p_2)|\, A^\mu_{4\mp i5}(0)\, |K^\pm(p_3+\vartheta_{K^\pm})\rangle &= \\ = \tfrac{\hat{m}+m_s}{2}\, \langle\pi_c(p_1)\pi_c(p_2)|\, P_{4\mp i5}(0)\, |K^\pm(p_3+\vartheta_{K^\pm})\rangle&\end{aligned} \tag{3.139c}$$

$$\begin{aligned}-i(\tilde{Q}+\vartheta_{K^0})_\mu \langle\pi_c(p_1)\pi_c(p_2)|\, A^\mu_{6-i7}(0)\, |K^0(p_3+\vartheta_{K^0})\rangle &= \\ = \tfrac{\hat{m}+m_s}{2}\, \langle\pi_c(p_1)\pi_c(p_2)|\, P_{6-i7}(0)\, |K^0(p_3+\vartheta_{K^0})\rangle&\end{aligned} \tag{3.139d}$$

$$\begin{aligned}-i\tilde{Q}_\mu \langle\pi_c(p_1)\pi_c(p_2)|\, A_8^\mu(0)\, |\eta(p_3)\rangle = \tfrac{\hat{m}+2m_s}{3}\, &\langle\pi_c(p_1)\pi_c(p_2)|\, P_8(0)\, |\eta(p_3)\rangle \\ + \sqrt{2}\, \tfrac{\hat{m}-m_s}{3}\, &\langle\pi_c(p_1)\pi_c(p_2)|\, P_0(0)\, |\eta(p_3)\rangle\, .\end{aligned} \tag{3.139e}$$

Here, the matrix elements are in infinite volume though momenta are shifted by the twisting angles. These matrix elements will provide us with the amplitudes entering the asymptotic formulae (3.99, 3.128). Note that $\langle\pi_c(p_1)\pi_c(p_2)|$ is a two-pion state with a zero isospin. We can leave out the twisting angles of that state as they will appear in the phase factors (3.148) after a substitution of the loop momentum like Eq. (3.32). On left-hand side, the momentum $\tilde{Q}^\mu = (p_3 - p_2 - p_1)^\mu$ is defined as before and will be set on-shell by the pole subtraction. For convenience, we detail here just the demonstration of charged pions. The relations of other pseudoscalar mesons can be demonstrated in an analogous way.

We rewrite the chiral Ward identities (3.139b) in a compact notation as

$$-i\left(\tilde{Q}+\vartheta_{\pi^\pm}\right)_\mu \left(A_{\pi^\pm\pi_c}(\vartheta_{\pi^\pm})\right)^\mu = \hat{m}\, C_{\pi^\pm\pi_c}(\vartheta_{\pi^\pm}), \tag{3.140}$$

where

$$\begin{aligned}\left(A_{\pi^\pm\pi_c}(\vartheta_{\pi^\pm})\right)^\mu &= \langle\pi_c(p_1)\pi_c(p_2)|\, A^\mu_{1\mp i2}(0)\, |\pi^\pm(p_3+\vartheta_{\pi^\pm})\rangle \\ C_{\pi^\pm\pi_c}(\vartheta_{\pi^\pm}) &= \langle\pi_c(p_1)\pi_c(p_2)|\, P_{1\mp i2}(0)\, |\pi^\pm(p_3+\vartheta_{\pi^\pm})\rangle\, .\end{aligned} \tag{3.141}$$

According to Ref. [47] the matrix elements $\left(A_{\pi^\pm\pi_c}(\vartheta_{\pi^\pm})\right)^\mu$ have a pole that does not enter in the amplitudes of the asymptotic formulae. We subtract the pole expanding the matrix elements around $(\tilde{Q}+\vartheta_{\pi^\pm})^2 = M_\pi^2$,

$$\begin{aligned}\left(A_{\pi^\pm\pi_c}(\vartheta_{\pi^\pm})\right)^\mu &= \left(\bar{A}_{\pi^\pm\pi_c}(\vartheta_{\pi^\pm})\right)^\mu \\ &+ iF_\pi(\tilde{Q}+\vartheta_{\pi^\pm})^\mu \frac{T_{\pi^\pm\pi_c}\big(s(\vartheta_{\pi^\pm}), t(\vartheta_{\pi^\pm}) - u(\vartheta_{\pi^\pm})\big)}{M_\pi^2 - (\tilde{Q}+\vartheta_{\pi^\pm})^2}.\end{aligned} \tag{3.142}$$

Here, $T_{\pi^\pm\pi_c}\big(s(\vartheta_{\pi^\pm}), t(\vartheta_{\pi^\pm}) - u(\vartheta_{\pi^\pm})\big)$ correspond to the isospin components (3.81) and

$$\begin{aligned} s(\vartheta_{\pi^\pm}) &= \Big[\tilde{Q} + \vartheta_{\pi^\pm} - (p_3 + \vartheta_{\pi^\pm})\Big]^2 \\ t(\vartheta_{\pi^\pm}) &= (\tilde{Q} + \vartheta_{\pi^\pm} + p_2)^2 \\ u(\vartheta_{\pi^\pm}) &= (\tilde{Q} + \vartheta_{\pi^\pm} + p_1)^2, \end{aligned} \tag{3.143}$$

are the Mandelstam variables (3.14) shifted by the twisting angles of p_3, $\tilde{Q}$. We observe that the first variable does not depend on $\vartheta^\mu_{\pi^\pm}$ as twisting angles exactly cancel out: $s(\vartheta_{\pi^\pm}) = s$. The bar indicates that the pole has been subtracted from the matrix elements. This means that $\big(\bar{A}_{\pi^\pm\pi_c}(\vartheta_{\pi^\pm})\big)^\mu$ correspond to the matrix elements (3.109) with p_3, $\tilde{Q}$ shifted by the twisting angles $\vartheta^\mu_{\pi^\pm}$.

Similarly, the matrix elements $C_{\pi^\pm\pi_c}(\vartheta_{\pi^\pm})$ have a pole that does not enter in the amplitudes of the asymptotic formulae, see Ref. [31]. We subtract the pole expanding the matrix elements around $(\tilde{Q} + \vartheta_{\pi^\pm})^2 = M_\pi^2$,

$$C_{\pi^\pm\pi_c}(\vartheta_{\pi^\pm}) = \bar{C}_{\pi^\pm\pi_c}(\vartheta_{\pi^\pm}) + G_\pi \frac{T_{\pi^\pm\pi_c}\big(s, t(\vartheta_{\pi^\pm}) - u(\vartheta_{\pi^\pm})\big)}{M_\pi^2 - (\tilde{Q} + \vartheta_{\pi^\pm})^2}. \tag{3.144}$$

Note that $\bar{C}_{\pi^\pm\pi_c}(\vartheta_{\pi^\pm})$ correspond to the matrix elements (3.131) with p_3, $\tilde{Q}$ shifted by $\vartheta^\mu_{\pi^\pm}$.

We insert the expansions (3.142, 3.144) in the identities (3.140) and divide for M_π. Using $\hat{m}G_\pi = M_\pi^2 F_\pi$ we find

$$-\frac{i}{M_\pi}\left(\tilde{Q} + \vartheta_{\pi^\pm}\right)_\mu \big(\bar{A}_{\pi^\pm\pi_c}(\vartheta_{\pi^\pm})\big)^\mu = \frac{\hat{m}}{M_\pi}\,\bar{C}_{\pi^\pm\pi_c}(\vartheta_{\pi^\pm}) + \frac{F_\pi}{M_\pi}\,T_{\pi^\pm\pi_c}\big(s_3, s_1(\vartheta_{\pi^\pm}) - s_2(\vartheta_{\pi^\pm})\big). \tag{3.145}$$

The last term can be brought on the left-hand side. We set $p_1^\mu = -p_2^\mu = k^\mu$ and rewrite the momenta $(p_3 + \vartheta_{\pi^\pm})^\mu = (\hat{p} + \hat{\vartheta}_{\pi^\pm})^\mu$ as in Eq. (3.55). We obtain

$$-\frac{i}{M_\pi}\,(\hat{p} + \hat{\vartheta}_{\pi^\pm})_\mu \big(\bar{A}_{\pi^\pm\pi_c}(\hat{\vartheta}_{\pi^\pm})\big)^\mu - \frac{F_\pi}{M_\pi}\,T_{\pi^\pm\pi_c}\big(0, -4M_\pi\nu_\pm\big) = \frac{\hat{m}}{M_\pi}\,\bar{C}_{\pi^\pm\pi_c}(\hat{\vartheta}_{\pi^\pm}), \tag{3.146}$$

where $\nu_\pm = [u(\hat{\vartheta}_{\pi^\pm}) - t(\hat{\vartheta}_{\pi^\pm})]/(4M_\pi) = \nu + k_\mu\hat{\vartheta}^\mu_{\pi^\pm}/M_\pi$. Now, we expand for small external twisting angles (i.e. around $\hat{\vartheta}^\mu_{\pi^\pm} = 0$ or equivalently around $\nu_\pm = \nu$) and multiply both sides for

$$\frac{1}{2}\sum_{\substack{\vec{n}\in\mathbb{Z}^3 \\ |\vec{n}|\neq 0}} \int_{\mathbb{R}^4} \frac{\mathrm{d}^4 k}{(2\pi)^4}\,\mathrm{e}^{iL\vec{n}\vec{k}}\,\frac{\Omega_c}{M_\pi^2 + k^2}, \tag{3.147}$$

where

$$\Omega_c = \begin{cases} \exp(-iL\vec{n}\vec{\vartheta}_{\pi^+}), & \text{for} \quad c = 1 \\ \exp(-iL\vec{n}\vec{\vartheta}_{\pi^-}), & \text{for} \quad c = 2 \\ 1, & \text{for} \quad c = 3. \end{cases} \tag{3.148}$$

The contour integration of Fig. 3.3 provides us with the relations

$$\delta G_{\pi^\pm} - 2\,\hat{\vec{\vartheta}}_{\pi^\pm}\Delta\vec{\vartheta}_{\mathscr{G}_{\pi^\pm}} = 2\,\delta M_{\pi^\pm} + \delta F_{\pi^\pm} - \frac{2}{M_\pi^2}\,\hat{\vec{\vartheta}}_{\pi^\pm}\left(\Delta\vec{\vartheta}_{\mathscr{A}_{\pi^\pm}} - \Delta\vec{\vartheta}_{\Sigma_{\pi^\pm}}\right) + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}}). \quad (3.149)$$

Here, $\delta M_{\pi^\pm}$, $\delta F_{\pi^\pm}$, $\delta G_{\pi^\pm}$ resp. $\Delta\vec{\vartheta}_{\Sigma_{\pi^\pm}}$, $\Delta\vec{\vartheta}_{\mathscr{A}_{\pi^\pm}}$, $\Delta\vec{\vartheta}_{\mathscr{G}_{\pi^\pm}}$ are given in terms of asymptotic formulae. Obviously, these relations hold if the amplitudes entering the asymptotic formulae satisfy the conditions

$$\begin{aligned} \frac{\hat{m}}{M_\pi}\,\mathcal{C}_{\pi^\pm}(\tilde{\nu},\vartheta_{\pi^+}) &= \mathcal{N}_{\pi^\pm}(\tilde{\nu},\vartheta_{\pi^+}) - \frac{F_\pi}{M_\pi}\,\mathcal{F}_{\pi^\pm}(\tilde{\nu},\vartheta_{\pi^+}) \\ \frac{\hat{m}}{M_\pi}\,\mathcal{K}_{\pi^\pm}(\tilde{\nu},\vartheta_{\pi^+}) &= \mathcal{H}_{\pi^\pm}(\tilde{\nu},\vartheta_{\pi^+}) - \frac{F_\pi}{M_\pi}\,\mathcal{G}_{\pi^\pm}(\tilde{\nu},\vartheta_{\pi^+}). \end{aligned} \quad (3.150)$$

As check we compare the amplitudes on the left-hand side with the amplitudes on the right-hand side by means of the chiral representation. We use Eq. (16.4) of Ref. [10] to calculate $\mathcal{C}_{\pi^\pm}(\tilde{\nu},\vartheta_{\pi^+})$, $\mathcal{K}_{\pi^\pm}(\tilde{\nu},\vartheta_{\pi^+})$ and the results of Ref. [44,47] to calculate $\mathcal{F}_{\pi^\pm}(\tilde{\nu},\vartheta_{\pi^+})$, $\mathcal{G}_{\pi^\pm}(\tilde{\nu},\vartheta_{\pi^+})$ resp. $\mathcal{N}_{\pi^\pm}(\tilde{\nu},\vartheta_{\pi^+})$, $\mathcal{H}_{\pi^\pm}(\tilde{\nu},\vartheta_{\pi^+})$. We find that the expressions agree on both sides. Thus, in ChPT the conditions (3.150) are satisfied at NLO.

The relations for other pseudoscalar mesons can be demonstrated in an analogous way. Altogether, we obtain

$$\delta G_{\pi^0} = 2\,\delta M_{\pi^0} + \delta F_{\pi^0} + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}})$$

$$\begin{aligned} \delta G_{K^\pm} - 2\,\hat{\vec{\vartheta}}_{K^\pm}\Delta\vec{\vartheta}_{\mathscr{G}_{K^\pm}} &= 2\,\delta M_{K^\pm} + \delta F_{K^\pm} \\ &\qquad - \frac{2}{M_K^2}\,\hat{\vec{\vartheta}}_{K^\pm}\left(\Delta\vec{\vartheta}_{\mathscr{A}_{K^\pm}} - \Delta\vec{\vartheta}_{\Sigma_{K^\pm}}\right) + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}}) \\ \delta G_{K^0} - 2\,\hat{\vec{\vartheta}}_{K^0}\Delta\vec{\vartheta}_{\mathscr{G}_{K^0}} &= 2\,\delta M_{K^0} + \delta F_{K^0} \\ &\qquad - \frac{2}{M_K^2}\,\hat{\vec{\vartheta}}_{K^0}\left(\Delta\vec{\vartheta}_{\mathscr{A}_{K^0}} - \Delta\vec{\vartheta}_{\Sigma_{K^0}}\right) + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}}) \end{aligned} \quad (3.151)$$

$$\tfrac{\hat{m}+2m_s}{3}\,\frac{G_\eta}{M_\eta^2 F_\eta}\,\delta G_\eta = 2\,\delta M_\eta + \delta F_\eta - \frac{\sqrt{2}}{M_\eta^2 F_\eta}\,\tfrac{\hat{m}-m_s}{3}\,\Delta G_{0,\eta} + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}}).$$

Here, all corrections and renormalization terms are given through asymptotic formulae. Note that the relation for the eta meson exhibits an additional term, namely $\Delta G_{0,\eta}$. In Section 2.3.3 we have calculated this term at NLO in ChPT, see Eq. (2.69). In this case, it is given by the asymptotic formula,

$$\begin{aligned} \Delta G_{0,\eta} &= \langle 0|\,P_0\,|\eta\rangle_L - \langle 0|\,P_0\,|\eta\rangle \\ &= \frac{1}{(4\pi)^2}\frac{M_\pi^2}{\lambda_\pi}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\int_{\mathbb{R}}\frac{\mathrm{d}y}{|\vec{n}|}\,\mathrm{e}^{-\lambda_\pi|\vec{n}|\sqrt{1+y^2}}\,\mathcal{C}_{0,\eta}(iy,\vartheta_{\pi^+}) + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}}), \end{aligned} \quad (3.152)$$

where

$$\mathcal{C}_{0,\eta}(\tilde{\nu},\vartheta_{\pi^+}) = \bar{C}_{0,\eta\pi^0}(0,-4M_\eta\nu) + \left[\bar{C}_{0,\eta\pi^+}(0,-4M_\eta\nu) + \bar{C}_{0,\eta\pi^-}(0,-4M_\eta\nu)\right] \mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}. \quad (3.153)$$

The functions $\bar{C}_{0,\eta\pi^0}(s,t-u)$, $\bar{C}_{0,\eta\pi^+}(s,t-u)$, $\bar{C}_{0,\eta\pi^-}(s,t-u)$ can be determined from

$$\begin{aligned} C_{0,\eta\pi^0} &= \left\langle \pi^0(p_1)\pi^0(p_2)\right| P_0(0)\left|\eta(p_3)\right\rangle \\ C_{0,\eta\pi^+} &= \left\langle \pi^+(p_1)\pi^-(p_2)\right| P_0(0)\left|\eta(p_3)\right\rangle \\ C_{0,\eta\pi^-} &= \left\langle \pi^-(p_1)\pi^+(p_2)\right| P_0(0)\left|\eta(p_3)\right\rangle, \end{aligned} \quad (3.154)$$

after the pole subtraction

$$\begin{aligned} \bar{C}_{0,\eta\pi^0}(s,t-u) &= C_{0,\eta\pi^0} - G_{0,\eta}\frac{T_{\eta\pi^0}(s,t-u)}{M_\eta^2-\tilde{Q}^2} \\ \bar{C}_{0,\eta\pi^+}(s,t-u) &= C_{0,\eta\pi^+} - G_{0,\eta}\frac{T_{\eta\pi^+}(s,t-u)}{M_\eta^2-\tilde{Q}^2} \\ \bar{C}_{0,\eta\pi^-}(s,t-u) &= C_{0,\eta\pi^-} - G_{0,\eta}\frac{T_{\eta\pi^-}(s,t-u)}{M_\eta^2-\tilde{Q}^2}. \end{aligned} \quad (3.155)$$

The function $T_{\eta\pi^0}(s,t-u)$, $T_{\eta\pi^+}(s,t-u)$, $T_{\eta\pi^-}(s,t-u)$ correspond to the isospin components (3.87) in the s-channel. The matrix element $G_{0,\eta} = \langle 0|\, P_0\,|\eta\rangle$ is in infinite volume and is evaluated at NLO in Eq. (1.87).

The relations (3.151) hold if the amplitudes entering the asymptotic formulae satisfy the conditions

$$\begin{aligned} \frac{\hat{m}}{M_\pi}\,\mathcal{C}_{\pi^0}(\tilde{\nu},\vartheta_{\pi^+}) &= \mathcal{N}_{\pi^0}(\tilde{\nu},\vartheta_{\pi^+}) - \frac{F_\pi}{M_\pi}\,\mathcal{F}_{\pi^0}(\tilde{\nu},\vartheta_{\pi^+}) \\ \frac{\hat{m}+m_s}{2\,M_K}\,\mathcal{C}_{K^\pm}(\tilde{\nu},\vartheta_{\pi^+}) &= \mathcal{N}_{K^\pm}(\tilde{\nu},\vartheta_{\pi^+}) - \frac{F_K}{M_K}\,\mathcal{F}_{K^\pm}(\tilde{\nu},\vartheta_{\pi^+}) \\ \frac{\hat{m}+m_s}{2\,M_K}\,\mathcal{K}_{K^\pm}(\tilde{\nu},\vartheta_{\pi^+}) &= \mathcal{H}_{K^\pm}(\tilde{\nu},\vartheta_{\pi^+}) - \frac{F_K}{M_K}\,\mathcal{G}_{K^\pm}(\tilde{\nu},\vartheta_{\pi^+}) \\ \frac{\hat{m}+m_s}{2\,M_K}\,\mathcal{C}_{K^0}(\tilde{\nu},\vartheta_{\pi^+}) &= \mathcal{N}_{K^0}(\tilde{\nu},\vartheta_{\pi^+}) - \frac{F_K}{M_K}\,\mathcal{F}_{K^0}(\tilde{\nu},\vartheta_{\pi^+}) \\ \frac{\hat{m}+m_s}{2\,M_K}\,\mathcal{K}_{K^0}(\tilde{\nu},\vartheta_{\pi^+}) &= \mathcal{H}_{K^0}(\tilde{\nu},\vartheta_{\pi^+}) - \frac{F_K}{M_K}\,\mathcal{G}_{K^0}(\tilde{\nu},\vartheta_{\pi^+}) \\ \frac{\hat{m}+2m_s}{3\,M_\eta}\,\mathcal{C}_{\eta}(\tilde{\nu},\vartheta_{\pi^+}) &= \mathcal{N}_{\eta}(\tilde{\nu},\vartheta_{\pi^+}) - \frac{F_\eta}{M_\eta}\,\mathcal{F}_{\eta}(\tilde{\nu},\vartheta_{\pi^+}) - \frac{\sqrt{2}}{M_\eta}\frac{\hat{m}-m_s}{3}\,\mathcal{C}_{0,\eta}(\tilde{\nu},\vartheta_{\pi^+}). \end{aligned} \quad (3.156)$$

From these conditions we can determine unknown amplitudes if we know the explicit representation of the related amplitudes. For instance, we can determine $\mathcal{N}_{\pi^0}(\tilde{\nu},\vartheta_{\pi^+})$ from the chiral representation of $\mathcal{F}_{\pi^0}(\tilde{\nu},\vartheta_{\pi^+})$, $\mathcal{C}_{\pi^0}(\tilde{\nu},\vartheta_{\pi^+})$ or we can determine $\mathcal{C}_{K^\pm}(\tilde{\nu},\vartheta_{\pi^+})$

[resp. $\mathcal{K}_{K^\pm}(\tilde{\nu}, \vartheta_{\pi^+})$] from the chiral representation of $\mathcal{F}_{K^\pm}(\tilde{\nu}, \vartheta_{\pi^+})$, $\mathcal{N}_{K^\pm}(\tilde{\nu}, \vartheta_{\pi^+})$ [resp. $\mathcal{G}_{K^\pm}(\tilde{\nu}, \vartheta_{\pi^+})$, $\mathcal{H}_{K^\pm}(\tilde{\nu}, \vartheta_{\pi^+})$]. At tree level we find

$$
\begin{aligned}
\mathcal{N}_{\pi^0}(\tilde{\nu}, \vartheta_{\pi^+}) &= -2\, \frac{M_\pi}{F_\pi}\, \mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}, \\
\mathcal{C}_{K^\pm}(\tilde{\nu}, \vartheta_{\pi^+}) &= -\frac{G_K}{4F_\pi F_K} \left(1 + 2\mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}\right) \\
\mathcal{K}_{K^\pm}(\tilde{\nu}, \vartheta_{\pi^+}) &= \mp 2\, \frac{M_\pi}{F_\pi} \underbrace{\left[1 - \frac{F_K}{F_\pi}\right]}_{=0+\mathcal{O}(\xi_\pi)} \tilde{\nu}\, \mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}.
\end{aligned}
\tag{3.157}
$$

Inserting these amplitudes in the asymptotic formulae (3.99a, 3.128c, 3.132b) we obtain the results (2.75b, 2.58) if the contributions of virtual kaons and eta meson are discarded. Note that $\mathcal{K}_{K^\pm}(\tilde{\nu}, \vartheta_{\pi^+}) = 0 + \mathcal{O}(\xi_\pi M_\pi/F_\pi)$. This means that the renormalization terms $\Delta\vartheta^\mu_{\mathscr{G}_{K^\pm}}$ are not present at this order: they will appear from NNLO onwards.

3.5 Asymptotic Formulae for Pion Form Factors

3.5.1 Vanishing Momentum Transfer

As proposed by Häfeli [120] we can rely on the Feynman–Hellman Theorem to derive asymptotic formulae for the matrix elements of the scalar form factor. In Section 2.3.4 we have seen that in finite volume the Feynman–Hellman Theorem relates the corrections of the matrix elements of the scalar form factor with the derivative of the self energies. Extending Eqs. (2.88, 2.91) to higher orders we have

$$
\begin{aligned}
\delta\Gamma_S^{\pi^0}\big|_{q^2=0} &= \partial_{M_\pi^2}\left[-\Delta\Sigma_{\pi^0}\right] \\
\delta\Gamma_S^{\pi^\pm}\big|_{q^2=0} &= \partial_{M_\pi^2}\left[-\Delta\Sigma_{\pi^\pm}\right].
\end{aligned}
\tag{3.158}
$$

The self energies $\Delta\Sigma_{\pi^0}$, $\Delta\Sigma_{\pi^\pm}$ are on the mass shell in finite volume and $\partial_{M_\pi^2} = \partial/\partial M_\pi^2$. Starting from these relations we derive asymptotic formulae valid at a vanishing momentum transfer (i.e. for $q^2 = 0$).

In Section 3.2.2 the asymptotic formulae for the masses of pions were derived relying on Eqs. (3.27, 3.54). We can solve these equations with respect to the self energies where for charged pions we additionally use Eq. (3.77). We obtain

$$
\begin{aligned}
\Delta\Sigma_{\pi^0} &= -2M_\pi^2\, \delta M_{\pi^0} + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}}) \\
\Delta\Sigma_{\pi^\pm} &= -2M_\pi^2\, \delta M_{\pi^\pm} - 2\vec{\vartheta}_{\pi^\pm}\Delta\vec{\vartheta}_{\Sigma_{\pi^\pm}} + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}}).
\end{aligned}
\tag{3.159}
$$

Here, δM_{π^0}, $\delta M_{\pi^\pm}$, $\Delta\vec{\vartheta}_{\Sigma_{\pi^\pm}}$ are meant up to $\mathcal{O}(\mathrm{e}^{-\bar{\lambda}})$ where $\bar{\lambda} = \bar{M}L$ has the mass bound $\bar{M} = (\sqrt{3}+1)M_\pi/\sqrt{2}$. We insert these expressions in the initial relations and take the derivative $\partial_{M_\pi^2}$. We have

$$\begin{aligned}\delta\Gamma_S^{\pi^0}\big|_{q^2=0} &= 2\,\delta M_{\pi^0} + 2M_\pi^2\ \partial_{M_\pi^2}\delta M_{\pi^0} + \mathcal{O}(\mathrm{e}^{-\bar\lambda})\\ \delta\Gamma_S^{\pi^\pm}\big|_{q^2=0} &= 2\,\delta M_{\pi^\pm} + 2M_\pi^2\ \partial_{M_\pi^2}\delta M_{\pi^\pm} + 2\vec\vartheta_{\pi^\pm}\ \partial_{M_\pi^2}\Delta\vec\vartheta_{\Sigma_{\pi^\pm}} + \mathcal{O}(\mathrm{e}^{-\bar\lambda}).\end{aligned} \tag{3.160}$$

Since the formulae of δM_{π^0}, $\delta M_{\pi^\pm}$, $\Delta\vec\vartheta_{\Sigma_{\pi^\pm}}$ are known up to $\mathcal{O}(\mathrm{e}^{-\bar\lambda})$ we find the following asymptotic formulae,

$$\begin{aligned}\delta\Gamma_S^{\pi^0}\big|_{q^2=0} = &-\frac{1}{2\,(4\pi)^2\,\lambda_\pi}\sum_{\substack{\vec n\in\mathbb{Z}^3\\|\vec n|\neq 0}}\int_{\mathbb{R}}\frac{\mathrm{d}y}{|\vec n|}\ \mathrm{e}^{-\lambda_\pi|\vec n|\sqrt{1+y^2}}\\ &\times\left(1-\lambda_\pi|\vec n|\sqrt{1+y^2}+2M_\pi^2\partial_{M_\pi^2}\right)\mathcal{F}_{\pi^0}(iy,\vartheta_{\pi^+}) + \mathcal{O}(\mathrm{e}^{-\bar\lambda})\end{aligned} \tag{3.161a}$$

$$\begin{aligned}\delta\Gamma_S^{\pi^\pm}\big|_{q^2=0} = &-\frac{1}{2\,(4\pi)^2\,\lambda_\pi}\sum_{\substack{\vec n\in\mathbb{Z}^3\\|\vec n|\neq 0}}\int_{\mathbb{R}}\frac{\mathrm{d}y}{|\vec n|}\ \mathrm{e}^{-\lambda_\pi|\vec n|\sqrt{1+y^2}}\\ &\times\Bigg[\left(1-\lambda_\pi|\vec n|\sqrt{1+y^2}+2M_\pi^2\partial_{M_\pi^2}\right)\mathcal{F}_{\pi^\pm}(iy,\vartheta_{\pi^+})\\ &-y\,\frac{D_{\pi^\pm}}{M_\pi}\left(\lambda_\pi|\vec n|\sqrt{1+y^2}+\frac{M_\pi}{M_\pi+D_{\pi^\pm}}-2M_\pi^2\partial_{M_\pi^2}\right)\partial_y\mathcal{F}_{\pi^\pm}(iy,\vartheta_{\pi^+})\\ &+y\,L\vec n\vec\vartheta_{\pi^\pm}\left(1-\lambda_\pi|\vec n|\sqrt{1+y^2}+2M_\pi^2\partial_{M_\pi^2}\right)\mathcal{G}_{\pi^\pm}(iy,\vartheta_{\pi^+})\Bigg]+\mathcal{O}(\mathrm{e}^{-\bar\lambda}).\end{aligned} \tag{3.161b}$$

These asymptotic formulae estimate the corrections of the matrix elements of the scalar form factor at a vanishing momentum transfer. The formulae depend on the amplitudes defined in Eqs. (3.45, 3.80, 3.89a). Here, the dependence on the twist is threefold. The formulae depend on the twisting angle of the virtual positive pion through the phase factor $\exp(iL\vec n\vec\vartheta_{\pi^+})$ in the amplitudes. Furthermore, they depend on the external twisting angles through the parameter $D_{\pi^\pm}$ and through the product $\vec n\vec\vartheta_{\pi^\pm}$ in the last line of Eq. (3.161b). Note that the formulae for charged pions are valid for small external twisting angles. The formula for the neutral pion is valid for arbitrary twisting angles.

We check the above asymptotic formulae in two ways. First, we set all twisting angles to zero. We find

$$\begin{aligned}\delta\Gamma_S\big|_{q^2=0} = &-\frac{1}{2\,(4\pi)^2\,\lambda_\pi}\sum_{\substack{\vec n\in\mathbb{Z}^3\\|\vec n|\neq 0}}\int_{\mathbb{R}}\frac{\mathrm{d}y}{|\vec n|}\ \mathrm{e}^{-\lambda_\pi|\vec n|\sqrt{1+y^2}}\\ &\times\left(1-\lambda_\pi|\vec n|\sqrt{1+y^2}+2M_\pi^2\partial_{M_\pi^2}\right)\mathcal{F}_\pi(iy)+\mathcal{O}(\mathrm{e}^{-\bar\lambda}).\end{aligned} \tag{3.162}$$

This expression coincides with the formula originally proposed by Häfeli [120] and valid for PBC. In this case, $\mathcal{F}_\pi(\tilde\nu)$ is the amplitude entering the Lüscher formula for pions,

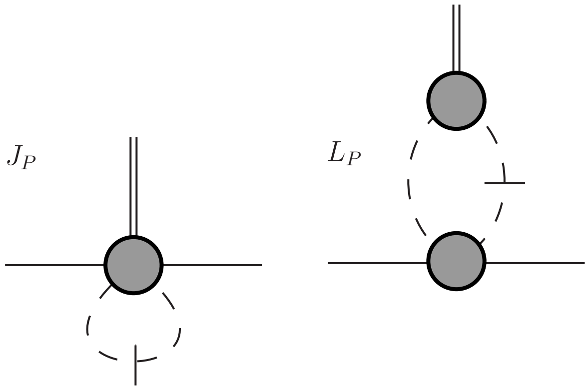


Figure 3.5: Skeleton diagrams contributing to asymptotic formulae for matrix elements of form factors. Solid lines stand for a generic pseudoscalar meson P and dashed lines for virtual pions. Double solid lines represent the scalar densities. The spline indicates that the pion propagator is in finite volume.

see Eq. (3.1). Second, we insert the chiral representation at tree level in the asymptotic formulae (3.161). The expressions obtained coincide with the results (2.86) found at NLO with 2-light-flavor ChPT.

3.5.2 Non-zero Momentum Transfer

The general derivation of asymptotic formulae for form factors is complicated by the presence of a non-zero momentum transfer. We anticipate that in this case we were not able to derive asymptotic formulae. However, we illustrate the steps undertaken and the complications encountered.

To keep the discussion simple, we focus on the scalar form factor and consider the matrix elements,

$$\langle \pi_b(p')|\, S_0(0)\, |\pi_a(p)\rangle \,, \tag{3.163}$$

in finite volume with TBC. In Appendix C.3 we show that these matrix elements behave like $\mathcal{O}(\mathrm{e}^{-\sqrt{3}\,\lambda_\pi/2})$ at asymptotically large L. The demonstration relies on Abstract Graph Theory and is similar to that of the self energies. It turns out that the dominant contribution is given by the diagrams of Fig. 3.5. The diagrams have an additional external double line representing the scalar densities. In principle, their contributions should be estimated with the contour integration in a similar way as in Section 3.2.2. In practice, the integration can not be performed as in Eq. (3.42) due to the presence of a non-zero momentum transfer introduced by the scalar densities.

To illustrate the complications encountered, we concentrate on the diagram L_P and consider P a neutral pion. Moreover, we choose the kinematics,

$$p^\mu = \hat{p}^\mu = \begin{bmatrix} iM_\pi \\ \vec{0} \end{bmatrix}, \quad p'^\mu = \begin{bmatrix} iE'_\pi \\ \vec{p}\,' \end{bmatrix} \quad \text{with} \quad E'_\pi = \sqrt{M_\pi^2 + |\vec{p}\,'|^2} \quad \text{and} \quad \vec{p}\,' = \tfrac{2\pi}{L}\left(\begin{smallmatrix} 1 \\ 0 \\ 0 \end{smallmatrix}\right). \tag{3.164}$$

In that kinematics the momentum transfer $q^\mu = (p' - p)^\mu$ has two non-zero components: the zeroth component $q_0 = i(E'_\pi - M_\pi)$ and the first spatial component $q_1 = 2\pi/L$. The diagram under consideration should be then estimated from the integral

$$L_{\pi^0} = \sum_{\substack{\vec{n}\in\mathbb{Z}^3 \\ |\vec{n}|\neq 0}} \int_{\mathbb{R}^4} \frac{\mathrm{d}^4 k}{(2\pi)^4}\, \mathrm{e}^{iL\vec{n}\vec{k}} \Big[\Xi_{\pi^0\pi^0} G_\pi(k) G_\pi(k+q) + \Xi_{\pi^0\pi^+} G_\pi(k+\vartheta_{\pi^+}) G_\pi(k+\vartheta_{\pi^+}+q) + \Xi_{\pi^0\pi^-} G_\pi(k+\vartheta_{\pi^-}) G_\pi(k+\vartheta_{\pi^-}+q) \Big]. \tag{3.165}$$

In this case, we directly account for all winding numbers $\vec{n} \in \mathbb{Z}^3$ with $|\vec{n}| \neq 0$. The propagators G_π are defined as in Eq. (3.31) and

$$\begin{aligned}
\Xi_{\pi^0\pi^0} &= \Gamma_{\pi^0\pi^0}(\hat{p}, k+q, -k, -p')\ \Lambda_{\pi^0}(-k-q, q, k) \\
\Xi_{\pi^0\pi^+} &= \Gamma_{\pi^0\pi^+}(\hat{p}, k+\vartheta_{\pi^+}+q, -k-\vartheta_{\pi^+}, -p')\ \Lambda_{\pi^+}(-k-\vartheta_{\pi^+}-q, q, k+\vartheta_{\pi^+}) \\
\Xi_{\pi^0\pi^-} &= \Gamma_{\pi^0\pi^+}(\hat{p}, k+\vartheta_{\pi^-}+q, -k-\vartheta_{\pi^-}, -p')\ \Lambda_{\pi^-}(-k-\vartheta_{\pi^-}-q, q, k+\vartheta_{\pi^-}),
\end{aligned} \tag{3.166}$$

are products of vertex functions. Note that positive (negative) momenta correspond to incoming (outgoing) pions. The vertex functions $\Gamma_{\pi^0\pi^0}$, $\Gamma_{\pi^0\pi^+}$, $\Gamma_{\pi^0\pi^+}$ are the same of Section 3.2.2. The vertex functions Λ_{π^0}, Λ_{π^+}, Λ_{π^-} are defined by the one-particle irreducible part of the amputated three-point function containing a scalar density and two interpolating fields of pions. In Ref. [23] Lüscher showed that such vertex functions can be analytically extended to a domain of the complex plane.

We substitute $k^\mu \mapsto k^\mu - \vartheta^\mu_{\pi^\pm}$ and write the integral as

$$L_{\pi^0} = \sum_{\substack{\vec{n}\in\mathbb{Z}^3 \\ |\vec{n}|\neq 0}} \int_{\mathbb{R}^4} \frac{\mathrm{d}^4 k}{(2\pi)^4}\, \mathrm{e}^{iL\vec{n}\vec{k}} G_\pi(k) G_\pi(k+q)\ \Xi \tag{3.167}$$

where

$$\Xi := \Big[\Xi_{\pi^0\pi^0} + \Xi_{\pi^0\pi^+} \mathrm{e}^{-iL\vec{n}\vec{\vartheta}_{\pi^+}} + \Xi_{\pi^0\pi^-} \mathrm{e}^{-iL\vec{n}\vec{\vartheta}_{\pi^-}} \Big]. \tag{3.168}$$

After the substitution, the vertex functions have all the same momentum dependence,

$$\begin{aligned}
\Xi_{\pi^0\pi^0} &= \Gamma_{\pi^0\pi^0}(\hat{p}, k+q, -k, -p')\ \Lambda_{\pi^0}(-k-q, q, k) \\
\Xi_{\pi^0\pi^+} &= \Gamma_{\pi^0\pi^+}(\hat{p}, k+q, -k, -p')\ \Lambda_{\pi^+}(-k-q, q, k) \\
\Xi_{\pi^0\pi^-} &= \Gamma_{\pi^0\pi^+}(\hat{p}, k+q, -k, -p')\ \Lambda_{\pi^-}(-k-q, q, k).
\end{aligned} \tag{3.169}$$

The product $G_\pi(k)G_\pi(k+q)$ can be expressed by means of the Feynman parametrization (A.4). Substituting $k^\mu \mapsto k^\mu - (1-z)q^\mu$ we have

$$L_{\pi^0} = \sum_{\substack{\vec{n}\in\mathbb{Z}^3 \\ |\vec{n}|\neq 0}} \int_0^1\!\!\int_{\mathbb{R}^4} \frac{\mathrm{d}z\ \mathrm{d}^4 k}{(2\pi)^4} \frac{\mathrm{e}^{iL\vec{n}\vec{k} - iL(1-z)\vec{n}\vec{q}}}{\left[M_z^2 + k^2\right]^2}\ \Xi\,, \tag{3.170}$$

where $M_z^2 = M_\pi^2 + z(z-1)q^2$ and $z \in [0,1]$ is the Feynman parameter. The momentum dependence of vertex functions is now given by

$$\Xi_{\pi^0\pi^0} = \Gamma_{\pi^0\pi^0}\big(\hat{p}, k+zq, -k+(1-z)q, -p'\big)\ \Lambda_{\pi^0}\big(-k-zq, q, k-(1-z)q\big), \qquad (3.171)$$

and similarly for $\Xi_{\pi^0\pi^+}$, $\Xi_{\pi^0\pi^-}$. Note that such momentum dependence can be expressed in terms of six Lorentz scalars (i.e. $\hat{p}^2$, q^2, $\hat{p}\cdot q$, k^2, $\hat{p}\cdot k$, $q\cdot k$) which are multiplied by non-negative powers of z.

We take a closer look to the expression (3.170). We observe that if we take the winding numbers belonging to

$$\mathbb{A}_1 = \left\{\vec{n} \in \mathbb{Z}^3 \mid \vec{n} = \begin{pmatrix} n_1 \\ 0 \\ 0 \end{pmatrix}, n_1 \neq 0\right\}, \qquad (3.172)$$

we may rotate $\vec{k} \in \mathbb{R}^3$ so that $\exp(iL\vec{n}\vec{k}) = \exp(iL|\vec{n}|k_1)$ without changing the rest of the integrand. This is a consequence of the kinematics chosen in Eq. (3.164). We decompose the integral in

$$L_{\pi^0} = L_{\pi^0}[\mathbb{A}_1] + L_{\pi^0}[\mathbb{Z}^3 \setminus \mathbb{A}_1], \qquad (3.173)$$

where $L_{\pi^0}[\mathbb{A}_1]$ is the part of the integral with winding numbers in $\mathbb{A}_1$ and $L_{\pi^0}[\mathbb{Z}^3 \setminus \mathbb{A}_1]$ is the rest. Denoting $\vec{k} = (k_1, k_\perp) \in \mathbb{R}^3$ we may rewrite the part with winding numbers in $\mathbb{A}_1$ as

$$\begin{aligned} L_{\pi^0}[\mathbb{A}_1] &= \int_{\mathbb{R}} \mathrm{d}k_1\, f(k_1) \\ f(k_1) &= \sum_{\substack{\vec{n}\in\mathbb{A}_1 \\ |\vec{n}|\neq 0}} \int_0^1\!\!\int_{\mathbb{R}^3} \frac{\mathrm{d}z\ \mathrm{d}k_0\ \mathrm{d}k_\perp}{(2\pi)^4} \frac{\mathrm{e}^{iL|\vec{n}|k_1 - iL(1-z)\vec{n}\vec{q}}}{\left[M_z^2 + k_0^2 + k_1^2 + k_\perp^2\right]^2}\ \Xi\,. \end{aligned} \qquad (3.174)$$

To estimate the k_1-integration we take k_1 in the complex plane and approximate the integration by the contour of Fig. 3.3. The integrand $f(k_1)$ exhibits two imaginary poles of the second order,

$$k_1^\pm = \pm i\sqrt{M_z^2 + k_0^2 + k_\perp^2}. \qquad (3.175)$$

The poles depend on k_0, $k_\perp$, z and will consequently move when we integrate over those variables. We observe that we can keep the upper pole k_1^+ within the contour of Fig. 3.3 if we restrict the values of k_0, $k_\perp$, z from $\mathbb{R}^3 \times [0,1]$ to

$$\mathbb{W} = \left\{(k_0, k_\perp, z) \in \mathbb{R}^3 \times [0,1] \mid k_0^2 + k_\perp^2 + 2M_\pi\left(E'_\pi - M_\pi\right) z(1-z) \leq \frac{5}{4} M_\pi^2\right\}. \qquad (3.176)$$

Obviously, this restriction affects the result of the k_1-integration but, because of the exponential factor $\exp(iL|\vec{n}|k_1)$ in the integrand $f(k_1)$, the net effect is $\mathcal{O}(\mathrm{e}^{-\bar{\lambda}})$ and hence, negligible.

By virtue of the Residue Theorem, we have

$$\int_{\gamma_1} f = 2\pi i\ \mathrm{Res}(f)_{k_1 = k_1^+} - \int_{\gamma_2} f - \int_{\gamma_3} f - \int_{\gamma_4} f. \qquad (3.177)$$

One can show that the integrals on the right-hand side are negligible. The argumentation is similar to that of Section 3.2.2. It results that the non-negligible contribution arises from the residue,

$$\begin{aligned}\mathrm{Res}(f)_{k_1=k_1^+} &= \lim_{k_1\to k_1^+}\frac{\mathrm{d}}{\mathrm{d}k_1}\left[(k_1-k_1^+)^2 f(k_1)\right]\\ &= \sum_{\substack{\vec{n}\in\mathbb{A}_1\\|\vec{n}|\neq 0}}\int_{\mathbb{W}}\frac{\mathrm{d}z\ \mathrm{d}k_0\ \mathrm{d}^2k_\perp}{(2\pi)^4}\,\frac{\mathrm{e}^{-L|\vec{n}||k_1^+|-iL\vec{n}\vec{q}(1-z)}}{4i|k_1^+|^2}\left[\left(L|\vec{n}|+\frac{1}{|k_1|}\right)\Xi-\frac{\mathrm{d}\Xi}{\mathrm{d}k_1}\right]_{k_1=k_1^+}.\end{aligned} \tag{3.178}$$

Note that the condition $k_1=k_1^+$ puts the loop momentum on the shell of the mass M_z:

$$k^2|_{k_1=k_1^+}=k_0^2+(k_1^+)^2+k_\perp^2=-M_z^2. \tag{3.179}$$

Hence, the momentum dependence of the vertex functions can be expressed in terms of the six Lorentz scalars,

$$\begin{aligned}\hat{p}^2 &= -M_\pi^2 & q^2 &= 2M_\pi(E_\pi'-M_\pi)\\ \hat{p}\cdot q &= M_\pi(M_\pi-E_\pi') & k^2 &= -M_z^2\\ \hat{p}\cdot k &= iM_\pi k_0 & q\cdot k &= i(E_\pi'-M_\pi)k_0+\tfrac{2\pi}{L}k_1^+.\end{aligned} \tag{3.180}$$

We rewrite the part of the integral with winding numbers in $\mathbb{A}_1$ as

$$\begin{aligned}L_{\pi^0}[\mathbb{A}_1] = \sum_{\substack{\vec{n}\in\mathbb{A}_1\\|\vec{n}|\neq 0}}\int_0^1\!\!\int_{\mathbb{R}^3}\frac{\mathrm{d}z\ \mathrm{d}k_0\ \mathrm{d}k_\perp}{(2\pi)^3}\,&\frac{\mathrm{e}^{-L|\vec{n}|\sqrt{M_z^2+k_0^2+k_\perp^2}-iL(1-z)\vec{n}\vec{q}}}{4\left(M_z^2+k_0^2+k_\perp^2\right)}\\ &\times\left[\left(L|\vec{n}|+\frac{1}{\sqrt{M_z^2+k_0^2+k_\perp^2}}\right)\Xi-\frac{\mathrm{d}\Xi}{\mathrm{d}k_1}\right]_{k_1=k_1^+}.\end{aligned}$$

Here, we have extended the integration from $\mathbb{W}$ to $\mathbb{R}^3\times[0,1]$ as the resulting effect is $\mathcal{O}(\mathrm{e}^{-\bar{\lambda}})$. The above expression is quite complicated to integrate. The vertex functions depend on the momenta according to Eq. (3.171). Setting $k_1=k_1^+$, the momentum dependence can be expressed in terms of the six Lorentz scalars listed in Eq. (3.180). In particular, we observe that –through the Lorentz scalar $q\cdot k$– the vertex functions depend on k_1^+ and hence, on $k_\perp$. This complicates the $k_\perp$-integration as one can not directly integrate as in Eq. (3.42). Moreover, the condition $k_1=k_1^+$ puts the loop momentum on the shell of the mass M_z. This confuses the identification of the vertex functions with physical on-shell amplitudes. We stress that these complications might be circumvented if one could expand the vertex functions around $q^2=0$. However, the discretization of $\vec{q}$ prevents one to perform such expansion and one must devise an alternative way.

The rest $L_{\pi^0}[\mathbb{Z}^3\setminus\mathbb{A}_1]$ is even more complicated to integrate. The winding numbers in $\mathbb{Z}^3\setminus\mathbb{A}_1$ have more than one spatial component different from zero. For these winding numbers and for the kinematics chosen, there is no spatial rotation so that $\exp(iL\vec{n}\vec{k}) = \exp(iL|\vec{n}|k_1)$ without changing the integrand of $L_{\pi^0}[\mathbb{Z}^3 \backslash \mathbb{A}_1]$. In particular, spatial rotations change the arguments of vertex functions through the Lorentz scalar $q \cdot k$. This complicates the integration on $k_\perp \in \mathbb{R}^2$ even more.

We conclude observing that the complications encountered here should not arise in matrix elements with two different external states, as e.g. $\langle K^+ | \, S_{4+i5} \, |\pi^0\rangle$. There, both external particles can be taken in the rest frame and the momentum transfer does not vanish. Then, the vertex functions can be expanded around small external angles and the integration performed in a similar way as Section 3.2.2. In principle, no further complications should arise in that case.

Chapter 4

Application of Asymptotic Formulae in ChPT

4.1 Chiral Representation of Amplitudes

We apply the asymptotic formulae derived in Chapter 3 in combination with ChPT and estimate finite volume corrections beyond NLO. For that purpose we need the chiral representation of the amplitudes at least at one-loop level. At that level the chiral representation is known for the most of the amplitudes presented in this work. In Tab. 4.1 we summarize all amplitudes and –if it is known– we give the review article containing the chiral representation at one loop. We also list the process from which the chiral representation can be determined. Note that $\mathcal{N}_{\pi^0}$, $\mathcal{C}_{K^\pm}$, $\mathcal{K}_{K^\pm}$ are unknown, but through Eq. (3.156) they can be calculated in terms of $\mathcal{F}_{\pi^0}$, $\mathcal{C}_{\pi^0}$; $\mathcal{F}_{K^\pm}$, $\mathcal{N}_{K^\pm}$ and $\mathcal{G}_{K^\pm}$, $\mathcal{H}_{K^\pm}$.

4.1.1 Chiral Representation at One Loop

Amplitudes of Pions

We first consider the amplitudes entering the asymptotic formulae for the pion masses and for the renormalization terms $\Delta\vartheta^{\mu}_{\Sigma_{\pi^\pm}}$. They are defined as

$$
\begin{aligned}
\mathcal{F}_{\pi^0}(\tilde{\nu},\vartheta_{\pi^+}) &= T_{\pi^0\pi^0}(0,-4M_\pi\nu) + \left[T_{\pi^0\pi^+}(0,-4M_\pi\nu) + T_{\pi^0\pi^-}(0,-4M_\pi\nu)\right] \mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}} \\
\mathcal{F}_{\pi^\pm}(\tilde{\nu},\vartheta_{\pi^+}) &= T_{\pi^\pm\pi^0}(0,-4M_\pi\nu) + \left[T_{\pi^\pm\pi^+}(0,-4M_\pi\nu) + T_{\pi^\pm\pi^-}(0,-4M_\pi\nu)\right] \mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}} \\
\mathcal{G}_{\pi^\pm}(\tilde{\nu},\vartheta_{\pi^+}) &= \left[T_{\pi^\pm\pi^+}(0,-4M_\pi\nu) - T_{\pi^\pm\pi^-}(0,-4M_\pi\nu)\right] \mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}.
\end{aligned}
\tag{4.1}
$$

The chiral representation of $\mathcal{F}_{\pi^0}$, $\mathcal{F}_{\pi^\pm}$, $\mathcal{G}_{\pi^\pm}$ can be determined from the $\pi\pi$-scattering,

$$
\pi(p_1) + \pi(p_2) \longrightarrow \pi(p_3) + \pi(p_4), \tag{4.2}
$$

in the forward kinematics. In ChPT the $\pi\pi$-scattering is given by means of the invariant amplitude $A(s,t,u)$ where s,t,u are the Mandelstam variables (3.14) in Minkowski space.

Table 4.1: Amplitudes entering asymptotic formulae, processes they describe and review articles containing the chiral representation at one loop. Here, $P_a \longrightarrow \pi_a(\pi_c\pi_c)$ denotes the pseudoscalar decay into three pions in which two pions form a state with a zero isospin.

Amplitude	Process	Ref.
$\mathcal{F}_{\pi^0}, \mathcal{F}_{\pi^\pm}, \mathcal{G}_{\pi^\pm}$	$\pi\pi$-scattering	[44]
$\mathcal{F}_{K^\pm}, \mathcal{G}_{K^\pm}, \mathcal{F}_{K^0}, \mathcal{G}_{K^0}$	$K\pi$-scattering	[45]
$\mathcal{F}_{\eta}$	$\eta\pi$-scattering	[46]
$\mathcal{N}_{\pi^0}$		
$\mathcal{N}_{\pi^\pm}, \mathcal{H}_{\pi^\pm}$	τ-decay	[47]
$\mathcal{N}_{K^\pm}, \mathcal{H}_{K^\pm}$	$K_{\ell 4}$-decay	[48]
$\mathcal{N}_{K^0}, \mathcal{H}_{K^0}$		
$\mathcal{N}_{\eta}$		
$\mathcal{C}_{\pi^0}, \mathcal{C}_{\pi^\pm}, \mathcal{K}_{\pi^\pm}$	$P_a \longrightarrow \pi_a(\pi_c\pi_c)$	[10]
$\mathcal{C}_{K^\pm}, \mathcal{K}_{K^\pm}$		
$\mathcal{C}_{K^0}, \mathcal{K}_{K^0}$		
$\mathcal{C}_{\eta}$		
$\mathcal{C}_{0,\eta}$		

The amplitude $A(s,t,u)$ is invariant under the interchange of the last two arguments, i.e. $A(s,t,u) = A(s,u,t)$ and is known up to NNLO in the chiral expansion, see Ref. [44]. As we want the chiral representation at one loop, we just need the part of $A(s,t,u)$ up to NLO. This was originally calculated in Ref. [10] and reads

$$
\begin{aligned}
A(s,t,u) = {} & \frac{s-M_\pi^2}{F_\pi^2} \\
& + \frac{1}{6F_\pi^4}\Bigg\{ -\frac{1}{N}\Bigg[+\frac{2}{3}\left(s+M_\pi^2\right)^2 + 2s^2 - 5M_\pi^4 + \frac{5}{6}\left[s^2+(t-u)^2\right]\Bigg] \\
& \qquad + \frac{1}{N}\Bigg[+2\bar{\ell}_1\left(s-2M_\pi^2\right)^2 + \bar{\ell}_2\left[s^2+(t-u)^2\right] - 3\bar{\ell}_3 M_\pi^4 \\
& \qquad\qquad + 12\bar{\ell}_4\left(s-M_\pi^2\right)M_\pi^2\Bigg] \\
& \qquad + 3\left(s^2-M_\pi^4\right)\bar{J}(s) + \Big[14M_\pi^4 + t(s+2t) - 2(2s+5t)M_\pi^2\Big]\bar{J}(t) \\
& \qquad + \Big[14M_\pi^4 + u(s+2u) - 2(2s+5u)M_\pi^2\Big]\bar{J}(u)\Bigg\}.
\end{aligned}
\tag{4.3}
$$

Here, $\bar{J}(t)$ is the loop-integral function defined in Eq. (D.19), $\bar{\ell}_j$ are the μ-independent constants introduced in Eq. (1.66) and $N = (4\pi)^2$. The isospin components of $\mathcal{F}_{\pi^0}$, $\mathcal{F}_{\pi^\pm}$,

$\mathcal{G}_{\pi^\pm}$ can be expressed in terms of the invariant amplitude $A_{stu} = A(s,t,u)$. They read

$$
\begin{aligned}
T_{\pi^0\pi^0}(t,u-s) &= A_{stu} + A_{tus} + A_{ust} \\[2ex]
T_{\pi^0\pi^+}(t,u-s) &= T_{\pi^0\pi^-}(t,u-s) \\
&= T_{\pi^+\pi^0}(t,u-s) \\
&= T_{\pi^-\pi^0}(t,u-s) = A_{tus} \\[2ex]
T_{\pi^+\pi^+}(t,u-s) &= T_{\pi^-\pi^-}(t,u-s) = A_{tus} + A_{ust} \\
T_{\pi^+\pi^-}(t,u-s) &= T_{\pi^-\pi^+}(t,u-s) = A_{stu} + A_{tus}.
\end{aligned}
\tag{4.4}
$$

The chiral representation of $\mathcal{F}_{\pi^0}$, $\mathcal{F}_{\pi^\pm}$, $\mathcal{G}_{\pi^\pm}$ can be obtained evaluating these expressions in the forward kinematics:

$$
s = 2M_\pi(M_\pi + \nu) \qquad t = 0 \qquad u = 2M_\pi(M_\pi - \nu). \tag{4.5}
$$

At tree level we find the results presented in Eq. (3.91).

The amplitudes $\mathcal{N}_{\pi^\pm}$ (resp. $\mathcal{H}_{\pi^\pm}$) entering the asymptotic formulae for the decay constants (resp. for the renormalization terms $\Delta\vartheta^\mu_{\mathscr{A}\pi^\pm}$) of charged pions are defined in Eqs. (3.100, 3.103). They can be determined from the matrix elements of the τ-decay,

$$
\tau(p_\tau) \longrightarrow \pi(p_1) + \pi(p_2) + \pi(p_3) + \nu_\tau(p_\tau - Q), \tag{4.6}
$$

in the forward kinematics, see Ref. [47]. In Section 3.3.2 we describe how to subtract the pole from these matrix elements in ChPT. Here, we just give the expressions of the factors entering the decomposition (3.105). Note that our expressions are a factor $1/\sqrt{2}$ smaller than the original ones of Ref. [47]. At NLO we have

$$
\begin{aligned}
F(s_1,s_2,s_3) &= iF_\pi \frac{A_{312}}{M_\pi^2 - Q^2} - \frac{i}{F_\pi}\left[1 - \frac{1}{F_\pi^2}\,\bar{F}^{(2)}(s_1,s_2,s_3)\right] \\
G(s_1,s_2,s_3) &= iF_\pi \frac{A_{312}}{M_\pi^2 - Q^2} + \frac{i}{F_\pi}\left[1 + \frac{1}{F_\pi^2}\,\bar{G}^{(2)}(s_1,s_2,s_3)\right] \\
H(s_1,s_2,s_3) &= \frac{i}{F_\pi^3}\,H^{(2)}(s_1,s_2,s_3).
\end{aligned}
\tag{4.7}
$$

Here, $A_{312} = A(s_3,s_1,s_2)$ is the invariant amplitude (4.3) reexpressed in terms of the variables s_1, s_2, s_3 of Eq. (3.106) and $Q^\mu = (p_1 + p_2 + p_3)^\mu$. The functions $\bar{F}^{(2)}(s_1,s_2,s_3)$,

$\bar{G}^{(2)}(s_1,s_2,s_3)$, $H^{(2)}(s_1,s_2,s_3)$ do not contain poles and are defined as

$$\begin{aligned}
\bar{F}^{(2)}(s_1,s_2,s_3) = &+\frac{M_\pi^2}{3}\left[\bar{J}(s_1)+\bar{J}(s_2)\right]-\frac{1}{12}(s_1-s_2)\left[\bar{J}(s_1)-\bar{J}(s_2)\right]-\frac{s_3}{2}\bar{J}(s_3)\\
&+\frac{1}{6N}\bigg[-2\bar{\ell}_1(s_3-2M_\pi^2)+\bar{\ell}_2(s_1+s_2+s_3-4M_\pi^2)-6\bar{\ell}_4M_\pi^2\\
&\qquad -\bar{\ell}_6(s_1+s_2+2s_3-4M_\pi^2)-\frac{1}{2}(s_1+s_2-5s_3)+\frac{8}{3}M_\pi^2\bigg]
\end{aligned}$$

$$\begin{aligned}
\bar{G}^{(2)}(s_1,s_2,s_3) = &-\frac{M_\pi^2}{6}\left[\bar{J}(s_1)+\bar{J}(s_2)\right]-\frac{1}{12}(s_1-s_2)\left[\bar{J}(s_1)-\bar{J}(s_2)\right]+\frac{s_3}{2}\bar{J}(s_3)\\
&+\frac{1}{6N}\bigg[+2\bar{\ell}_1(s_3-2M_\pi^2)-\bar{\ell}_2(s_1+s_2-s_3-4M_\pi^2)+6\bar{\ell}_4M_\pi^2\\
&\qquad +\bar{\ell}_6(s_1+s_2-2M_\pi^2)+\frac{1}{2}(s_1+s_2-7s_3)+\frac{10}{3}M_\pi^2\bigg]
\end{aligned} \tag{4.8}$$

$$\begin{aligned}
H^{(2)}(s_1,s_2,s_3) = &-\frac{1}{6}(s_1-s_2)\left[\bar{J}(s_1)+\bar{J}(s_2)\right]-\frac{1}{6}(s_1+s_2-5M_\pi^2)\left[\bar{J}(s_1)-\bar{J}(s_2)\right]\\
&-\frac{1}{6N}\bigg[\bar{\ell}_2(s_1-s_2)-\frac{5}{3}(s_1-s_2)\bigg].
\end{aligned}$$

One can convince oneself that the above expressions satisfy the properties (3.107). The chiral representation of $\mathcal{N}_{\pi^\pm}$, $\mathcal{H}_{\pi^\pm}$ can be obtained evaluating the isospin components (3.111) in the forward kinematics:

$$s_1 = 2M_\pi(M_\pi-\nu) \qquad s_2 = 2M_\pi(M_\pi+\nu) \qquad s_3 = 0. \tag{4.9}$$

At tree level we find the results presented in Eq. (3.114).

The amplitudes entering the asymptotic formulae for the pseudoscalar coupling constants of pions and for the renormalization terms $\Delta\vartheta^\mu_{\mathscr{G}_{\pi^\pm}}$ are defined as

$$\begin{aligned}
\mathcal{C}_{\pi^0}(\tilde{\nu},\vartheta_{\pi^+}) &= \bar{C}_{\pi^0\pi^0}(0,-4M_\pi\nu)\\
&\qquad +\left[\bar{C}_{\pi^0\pi^+}(0,-4M_\pi\nu)+\bar{C}_{\pi^0\pi^-}(0,-4M_\pi\nu)\right]\mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}\\
\mathcal{C}_{\pi^\pm}(\tilde{\nu},\vartheta_{\pi^+}) &= \bar{C}_{\pi^\pm\pi^0}(0,-4M_\pi\nu)\\
&\qquad +\left[\bar{C}_{\pi^\pm\pi^+}(0,-4M_\pi\nu)+\bar{C}_{\pi^\pm\pi^-}(0,-4M_\pi\nu)\right]\mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}\\
\mathcal{K}_{\pi^\pm}(\tilde{\nu},\vartheta_{\pi^+}) &= \left[\bar{C}_{\pi^\pm\pi^+}(0,-4M_\pi\nu)-\bar{C}_{\pi^\pm\pi^-}(0,-4M_\pi\nu)\right]\mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}.
\end{aligned} \tag{4.10}$$

These amplitudes can be determined from the point function containing four pseudoscalar densities, where three of them serve as interpolating fields for pions. In ChPT such point function can be calculated from Eq. (16.2) of Ref. [10]: one must take the off-shell amplitude $A(s,t,u;p_1^2,p_2^2,p_3^2,p_4^2)$ and set the momenta to $p_1^2 = p_2^2 = p_3^2 = M_\pi^2$ resp. $p_4^2 = \tilde{Q}^2$ where $\tilde{Q}^\mu = (p_3 - p_1 - p_2)^\mu$. Defining $C(s,t,u) = A(s,t,u;M_\pi^2,M_\pi^2,M_\pi^2,\tilde{Q}^2)$ we obtain

$$\begin{aligned}
C(s,t,u) = {} & \frac{s - M_\pi^2}{F_\pi} \\
& + \frac{1}{6F_\pi^4}\Bigg\{ -\frac{3}{N}\left[2s^2 - M_\pi^4 - (3s-t-u)M_\pi^2 - \frac{5}{9}\big[2tu - s(t+u)\big]\right] \\
& \qquad - \frac{1}{N}\Bigg[+ 2\bar{\ell}_1\left(s - 2M_\pi^2\right)\left(t + u - 2M_\pi^2\right) \\
& \qquad\qquad + 2\bar{\ell}_2\left[8M_\pi^4 + 2tu + s(t+u) - 4(s+t+u)M_\pi^2\right] \\
& \qquad\qquad + 3\bar{\ell}_3\left(s + t + u - 3M_\pi^2\right)M_\pi^2 \\
& \qquad\qquad - 6\bar{\ell}_4\left(s - M_\pi^2\right)\left(s + t + u - 2M_\pi^2\right)\Bigg] \\
& \qquad + 3\left(s - M_\pi^2\right)\left(2s + t + u - 3M_\pi^2\right)\bar{J}(s) \\
& \qquad - \left[6M_\pi^4 + (s+2u)t - (s+5u+3t)M_\pi^2\right]\bar{J}(t) \\
& \qquad - \left[6M_\pi^4 + (s+2t)u - (s+5t+3u)M_\pi^2\right]\bar{J}(u)\Bigg\}.
\end{aligned} \tag{4.11}$$

Note that the amplitude is invariant under the interchange of the last two arguments, i.e. $C(s,t,u) = C(s,u,t)$. The isospin components of $\mathcal{C}_{\pi^0}$, $\mathcal{C}_{\pi^\pm}$, $\mathcal{K}_{\pi^\pm}$ can be expressed in terms of $C_{stu} = C(s,t,u)$. They can be extracted from the following expressions,

$$\begin{aligned}
C_{\pi^0\pi^0}(s,t-u) &= \frac{G_\pi}{M_\pi^2 - \tilde{Q}^2}\left[C_{stu} + C_{tus} + C_{ust}\right] \\[2ex]
C_{\pi^0\pi^+}(s,t-u) &= C_{\pi^0\pi^-}(s,t-u) \\
&= C_{\pi^+\pi^0}(s,t-u) \\
&= C_{\pi^-\pi^0}(s,t-u) = \frac{G_\pi}{M_\pi^2 - \tilde{Q}^2}C_{stu} \\[2ex]
C_{\pi^+\pi^+}(s,t-u) &= C_{\pi^-\pi^-}(s,t-u) = \frac{G_\pi}{M_\pi^2 - \tilde{Q}^2}\left[C_{stu} + C_{tus}\right] \\
C_{\pi^+\pi^-}(s,t-u) &= C_{\pi^-\pi^+}(s,t-u) = \frac{G_\pi}{M_\pi^2 - \tilde{Q}^2}\left[C_{stu} + C_{ust}\right],
\end{aligned} \tag{4.12}$$

after having subtracted the pole at $\tilde{Q}^2 = M_\pi^2$. In Section 3.4.1 we describe how to subtract this pole and how to define the isospin components, see Eq. (3.131). The chiral representation can be obtained from that definition, evaluating the isospin components in the forward kinematics:

$$s = 0 \qquad t = 2M_\pi(M_\pi - \nu) \qquad u = 2M_\pi(M_\pi + \nu). \tag{4.13}$$

At tree level we find the results presented in Eq. (3.135).

In Section 3.5.1 we derive asymptotic formulae for the matrix elements of the scalar form factor of pions at a vanishing momentum transfer. The amplitudes entering these formulae are $\mathcal{F}_{\pi^0}$, $\mathcal{F}_{\pi^\pm}$, $\mathcal{G}_{\pi^\pm}$. The chiral representation is given by the isospin components (4.4) evaluated in the forward kinematics. In this case, the asymptotic formulae contain the derivatives $\partial_{M_\pi^2}\mathcal{F}_{\pi^0}$, $\partial_{M_\pi^2}\mathcal{F}_{\pi^\pm}$, $\partial_{M_\pi^2}\mathcal{G}_{\pi^\pm}$. One must pay some attention calculating these derivatives and let $\partial_{M_\pi^2}$ act on all quantities dependent on M_π contained in $\mathcal{F}_{\pi^0}$, $\mathcal{F}_{\pi^\pm}$, $\mathcal{G}_{\pi^\pm}$.

Amplitudes of Kaons

The amplitudes entering the asymptotic formulae for the kaon masses and for the renormalization terms $\Delta\vartheta^\mu_{\Sigma_{K^\pm}}$, $\Delta\vartheta^\mu_{\Sigma_{K^0}}$ are defined as

$$\begin{aligned}\mathcal{F}_{K^\pm}(\tilde{\nu}, \vartheta_{\pi^+}) &= T_{K^\pm\pi^0}(0, -4M_K\nu) \\ &\quad + \left[T_{K^\pm\pi^+}(0, -4M_K\nu) + T_{K^\pm\pi^-}(0, -4M_K\nu)\right] \mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}} \\ \mathcal{G}_{K^\pm}(\tilde{\nu}, \vartheta_{\pi^+}) &= \left[T_{K^\pm\pi^+}(0, -4M_K\nu) - T_{K^\pm\pi^-}(0, -4M_K\nu)\right] \mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}},\end{aligned} \tag{4.14}$$

where for $\mathcal{F}_{K^0}$, $\mathcal{G}_{K^0}$ hold similar expressions, see Eqs. (3.84, 3.89c). The chiral representation can be determined from the $K\pi$-scattering,

$$\pi^+(p_1) + K^+(p_2) \longrightarrow \pi^+(p_3) + K^+(p_4), \tag{4.15}$$

in the forward kinematics. In ChPT this scattering process is given by means of the amplitude $T^{3/2}(s,t,u)$ which is known up to NNLO, see Ref. [134]. Here, we just need the part up to NLO that was presented in Ref. [45]:

$$T^{3/2}(s,t,u) = T_2(s,t,u) + T_4^T(s,t,u) + T_4^P(s,t,u) + T_4^U(s,t,u). \tag{4.16}$$

The first term corresponds to the tree-level scattering,

$$T_2(s,t,u) = \frac{1}{2F_\pi}\left(M_\pi^2 + M_K^2 - s\right). \tag{4.17}$$

The second term contains contributions from the tadpole diagrams,

$$\begin{aligned}T_4^T(s,t,u) = \frac{1}{32NF_\pi^4}\Big[&+ \ell_\pi M_\pi^2\left(10s - 7M_\pi^2 - 13M_K^2\right) \\ &+ \ell_K M_K^2\left(2M_\pi^2 + 6M_K^2 - 4s\right) + \ell_\eta M_\eta^2\left(5M_\pi^2 + 7M_K^2 - 6s\right)\Big].\end{aligned} \tag{4.18}$$

Here, $N = (4\pi)^2$, $\ell_P = 2\log(M_P/\mu)$ for $P = \pi, K, \eta$ and μ is the renormalization scale. The third term originates from tree graphs at NLO and is a polynomial in s, t, u,

$$
\begin{aligned}
T_4^P(s,t,u) = \frac{2}{F_\pi^4}\Big\{ &+ 4L_1^{\mathrm{r}}\left(t-2M_\pi^2\right)\left(t-2M_K^2\right) \\
&+ 2L_2^{\mathrm{r}}\left[\left(s-M_\pi^2-M_K^2\right)^2+\left(u-M_\pi^2-M_K^2\right)^2\right] \\
&+ L_3^{\mathrm{r}}\left[\left(u-M_\pi^2-M_K^2\right)^2+\left(t-2M_\pi^2\right)\left(t-2M_K^2\right)\right] \\
&+ 4L_4^{\mathrm{r}}\left[t\left(M_\pi^2+M_K^2\right)-4M_\pi^2M_K^2\right] \\
&+ 2L_5^{\mathrm{r}}M_\pi^2\left(M_\pi^2-M_K^2-s\right)+8(2L_6^{\mathrm{r}}+L_8^{\mathrm{r}})M_\pi^2M_K^2\Big\}.
\end{aligned}
\tag{4.19}
$$

It includes the renormalized LEC L_j^{r} of Eq. (1.59). The last term contains unitarity corrections[1]

$$
\begin{aligned}
T_4^U(s,t,u) = \frac{1}{4F_\pi^4}\Bigg\{ &+ t(u-s)\left[2M_{\pi\pi}^r(t)+M_{KK}^r(t)\right] \\
&+ \frac{3}{2}\Big\{ + (s-t)\Big[L_{\pi K}(u)+L_{K\eta}(u)-u\left[M_{\pi K}^r(u)+M_{K\eta}^r(u)\right]\Big] \\
&\qquad + \left(M_K^2-M_\pi^2\right)^2\left[M_{\pi K}^r(u)+M_{K\eta}^r(u)\right]\Big\} \\
&+ \frac{1}{2}\left(M_K^2-M_\pi^2\right)\Big[+K_{\pi K}(u)\left(5u-2M_\pi^2-2M_K^2\right) \\
&\qquad\qquad + K_{K\eta}(u)\left(3u-2M_\pi^2-2M_K^2\right)\Big] \\
&+ J_{\pi K}^r(s)\left(s-M_\pi^2-M_K^2\right)^2 \\
&+ \frac{1}{8}J_{\pi K}^r(u)\left[11u^2-12u\left(M_K^2+M_\pi^2\right)+4\left(M_K^2+M_\pi^2\right)^2\right] \\
&+ \frac{3}{8}J_{K\eta}^r(u)\left[u-\frac{2}{3}\left(M_K^2+M_\pi^2\right)\right]^2+\frac{1}{2}J_{\pi\pi}^r(t)\,t\left(2t-M_\pi^2\right) \\
&+ \frac{3}{4}J_{KK}^r(t)\,t^2+\frac{1}{2}J_{\eta\eta}^r(t)M_\pi^2\left[t-\frac{8}{9}M_K^2\right]\Bigg\}.
\end{aligned}
\tag{4.20}
$$

Here, $J_{PQ}^r(t)$, $K_{PQ}(t)$, $L_{PQ}(t)$, $M_{PQ}^r(t)$ for $P, Q = \pi, K, \eta$ are loop-integral functions introduced in Ref. [11]. With the abbreviations,

$$
\begin{aligned}
J^r(t) &= J_{PQ}^r(t) & M &= M_P \\
K(t) &= K_{PQ}(t) & m &= M_Q \\
L(t) &= L_{PQ}(t) & \Delta &= M^2-m^2 \\
M^r(t) &= M_{PQ}^r(t) & k &= (M^2\ell_P-m^2\ell_Q)/(2N\Delta),
\end{aligned}
\tag{4.21}
$$

[1]As noted in [32] there are two missprints in Eq. (3.16) of [45]. The prefactor of $[M_{\pi K}^r(u)+M_{K\eta}^r(u)]$ should read $(M_K^2-M_\pi^2)^2$ and the factor of $\frac{3}{8}J_{K\eta}^r(u)$ should read $[u-\frac{2}{3}(M_\pi^2+M_K^2)]^2$.

they take the compact forms,

$$\begin{aligned} J^r(t) &= \bar{J}(t) - 2k \\ K(t) &= \frac{\Delta}{2t}\bar{J}(t) \\ L(t) &= \frac{\Delta^2}{4t}\bar{J}(t) \\ M^r(t) &= \bar{M}(t) - \frac{k}{6}. \end{aligned} \tag{4.22}$$

In Eq. (D.34) we give the expicit expressions of $\bar{J}(t) = \bar{J}_{PQ}(t)$ and $\bar{M}(t) = \bar{M}_{PQ}(t)$.

The isospin components of $\mathcal{F}_{K^\pm}$, $\mathcal{G}_{K^\pm}$ (as well as those of $\mathcal{F}_{K^0}$, $\mathcal{G}_{K^0}$) can be expressed in terms of the amplitude $T^{3/2}_{stu} = T^{3/2}(s,t,u)$. They read

$$\begin{aligned} T_{K^+\pi^0}(t,u-s) &= T_{K^-\pi^0}(t,u-s) \\ &= T_{K^0\pi^0}(t,u-s) = \frac{1}{2}\left[T^{3/2}_{stu} + T^{3/2}_{uts}\right] \\ \\ T_{K^+\pi^+}(t,u-s) &= T_{K^-\pi^-}(t,u-s) \\ &= T_{K^0\pi^-}(t,u-s) = T^{3/2}_{stu} \\ \\ T_{K^+\pi^-}(t,u-s) &= T_{K^-\pi^+}(t,u-s) \\ &= T_{K^0\pi^+}(t,u-s) = T^{3/2}_{uts}. \end{aligned} \tag{4.23}$$

The chiral representation of $\mathcal{F}_{K^\pm}$, $\mathcal{G}_{K^\pm}$ (resp. $\mathcal{F}_{K^0}$, $\mathcal{G}_{K^0}$) can be obtained evaluating these expressions in the forward kinematics:

$$s = M_K^2 + M_\pi^2 + 2M_K\nu \qquad t = 0 \qquad u = M_K^2 + M_\pi^2 - 2M_K\nu. \tag{4.24}$$

At tree level we find the results presented in Eq. (3.91).

Note that from the expressions (4.23) result that the isospin components of the negative kaon are equal to those of the neutral one. In this case, the chiral representation of the negative kaon corresponds to that of the neutral one. Thus, we have

$$\begin{aligned} \mathcal{F}_{K^0}(\tilde{\nu},\vartheta_{\pi^+}) &= \mathcal{F}_{K^-}(\tilde{\nu},\vartheta_{\pi^+}) \\ \mathcal{G}_{K^0}(\tilde{\nu},\vartheta_{\pi^+}) &= \mathcal{G}_{K^-}(\tilde{\nu},\vartheta_{\pi^+}). \end{aligned} \tag{4.25}$$

The amplitudes $\mathcal{N}_{K^\pm}$ (resp. $\mathcal{H}_{K^\pm}$) entering the asymptotic formulae for the decay constants (resp. for the renormalization terms $\Delta\vartheta^\mu_{\mathscr{A}_{K^\pm}}$) of charged kaons are defined in Eqs. (3.121, 3.123). They can be determined from the matrix elements of the $K_{\ell 4}$-decay,

$$K^+(p_3) \longrightarrow \pi(p_1) + \pi(p_2) + \ell^+(p_\ell) + \bar{\nu}_\ell(\tilde{Q} - p_\ell), \tag{4.26}$$

in the forward kinematics, see Ref. [48]. In Section 3.3.2 we describe how to subtract the pole from these matrix elements in ChPT. Here, we give the expressions of the factors entering the decomposition (3.117). Note that our expressions are a factors are $1/\sqrt{2}$ smaller than the original ones of Ref. [48]. At NLO we have

$$\begin{aligned}
F(s,t,u) &= \frac{M_K}{2F_\pi}\left\{1+\frac{1}{F_\pi^2}\left[C_F+P_F(s,t,u)+U_F(s,t,u)\right]\right\}\\
G(s,t,u) &= \frac{M_K}{2F_\pi}\left\{1+\frac{1}{F_\pi^2}\left[C_G+P_G(s,t,u)+U_G(s,t,u)\right]\right\}\\
R(s,t,u) &= \frac{M_K}{4F_\pi}\left\{1+\frac{1}{F_\pi^2}\left[C_Q+P_Q(s,t,u)+U_Q(s,t,u)\right]+\frac{Z(s,t,u)}{\tilde{Q}^2-M_K^2}\right\},
\end{aligned} \tag{4.27}$$

where

$$Z(s,t,u) = s+t-u+\frac{1}{F_\pi^2}\left[C_Z+P_Z(s,t,u)+U_Z(s,t,u)\right]. \tag{4.28}$$

The terms C_X (with $X=F,G,Q,Z$) do not depend on the Mandelstam variables s,t,u and contain the mass logarithms ℓ_P:

$$\begin{aligned}
C_F &= -C_G = 2\,C_Q\\
&= \frac{1}{16N}\left(5M_\pi^2\ell_\pi-2M_K^2\ell_K-3M_\eta^2\ell_\eta\right)\\
C_Z &= -\frac{M_K^2-M_\pi^2}{8N}\left(3M_\pi^2\ell_\pi-2M_K^2\ell_K-M_\eta^2\ell_\eta\right).
\end{aligned} \tag{4.29}$$

The terms $P_X(s,t,u)$ originate from tree graphs at NLO and are polynomials in s,t,u:

$$P_X(s,t,u) = \sum_{j=1}^{9} p_j^X(s,t,u)L_j^{\mathrm{r}}, \qquad X=F,G,Q,Z. \tag{4.30}$$

They include the renormalized LEC L_j^{r} of Eq. (1.59). The coefficients $p_j^X(s,t,u)$ are listed in Tab. 4.2 (resp. in Tab. 4.3) for $X=F,G,Q$ (resp. for $X=Z$). The terms $U_X(s,t,u)$ originate from one-loop diagrams and contain unitarity corrections. For $X=F,G$ they read

$$\begin{aligned}
U_F(s,t,u) &= \Delta_0(s)\\
&\quad+\frac{1}{16}\left[\left(14M_K^2+14M_\pi^2-19t\right)J_{K\pi}^r(t)+\left(2M_K^2+2M_\pi^2-3t\right)J_{\eta K}^r(t)\right]\\
&\quad+\frac{1}{8}\left[\left(3M_K^2-7M_\pi^2+5t\right)K_{K\pi}(t)+\left(M_K^2-5M_\pi^2+3t\right)K_{\eta K}(t)\right]\\
&\quad-\frac{1}{4}\left\{9\left[L_{K\pi}(t)+L_{\eta K}(t)\right]+3\left(M_K^2-M_\pi^2-3t\right)\left[M_{K\pi}^r(t)+M_{\eta K}^r(t)\right]\right\}\\
&\quad-\frac{1}{2}\left(M_K^2+M_\pi^2-t\right)J_{K\pi}^r(t)-\frac{1}{2}\left(M_K^2+M_\pi^2-u\right)J_{K\pi}^r(u),
\end{aligned} \tag{4.31}$$

and

$$
\begin{aligned}
U_G(s,t,u) &= \Delta_1(s) \\
&+ \frac{1}{16}\left[\left(2M_K^2+2M_\pi^2+3t\right) J^r_{K\pi}(t) - \left(2M_K^2+2M_\pi^2-3t\right) J^r_{\eta K}(t)\right] \\
&- \frac{1}{8}\left[\left(3M_K^2-7M_\pi^2+5t\right) K_{K\pi}(t) + \left(M_K^2-5M_\pi^2+3t\right) K_{\eta K}(t)\right] \\
&- \frac{3}{4}\Big\{L_{K\pi}(t)+L_{\eta K}(t) - \left(M_K^2-M_\pi^2+t\right)\left[M^r_{K\pi}(t)+M^r_{\eta K}(t)\right]\Big\}.
\end{aligned}
\tag{4.32}
$$

Here, $J^r_{PQ}(t)$, $K_{PQ}(t)$, $L_{PQ}(t)$, $M^r_{PQ}(t)$ are the loop-integral functions of Eq. (4.21) and

$$
\begin{aligned}
\Delta_0(s) &= \frac{1}{2}\left(2s-M_\pi^2\right) J^r_{\pi\pi}(s) + \frac{3}{4}\, s\ J^r_{KK}(s) + \frac{M_\pi^2}{2}\, J^r_{\eta\eta}(s) \\
\Delta_1(s) &= s\left[2M^r_{\pi\pi}(s)+M^r_{KK}(s)\right].
\end{aligned}
\tag{4.33}
$$

For $X = Q, Z$ the terms read

$$
\begin{aligned}
U_Q(s,t,u) &= \Delta_0(s) + \frac{M_K^2-\tilde{Q}^2}{32}\left[11J^r_{K\pi}(t)+8J^r_{K\pi}(u)+3J^r_{\eta K}(t)\right] \\
&- \frac{1}{8}\Big[5(s-t+u)+5\big(M_K^2-\tilde{Q}^2\big)-6\left(M_K^2+M_\pi^2\right)\Big] K_{K\pi}(t) \\
&- \frac{1}{8}\Big[3(s-t+u)+3\big(M_K^2-\tilde{Q}^2\big)-2\left(M_K^2+M_\pi^2\right)\Big] K_{\eta K}(t) \\
&- \frac{9}{4}\left[L_{K\pi}(t)+L_{\eta K}(t)\right] \\
&+ \frac{3}{8}\Big[4\left(t-u+2M_\pi^2\right)-3\big(M_K^2-\tilde{Q}^2\big)\Big]\left[M^r_{K\pi}(t)+M^r_{\eta K}(t)\right],
\end{aligned}
\tag{4.34}
$$

Table 4.2: Coefficients $p_j^F(s,t,u)$, $p_j^G(s,t,u)$ and $p_j^Q(s,t,u)$.

j	$p_j^F(s,t,u)$	$p_j^G(s,t,u)$	$p_j^Q(s,t,u)$
1	$32(s-2M_\pi^2)$		$32(s-2M_\pi^2)$
2	$8(M_K^2+s-\tilde{Q}^2)$	$8(t-u)$	$8(M_K^2-\tilde{Q}^2)$
3	$4(M_K^2-3M_\pi^2+2s-t)$	$4(t-M_K^2-M_\pi^2)$	$8(s-2M_\pi^2)+2(M_K^2-\tilde{Q}^2)$
4	$32M_\pi^2$		$32M_\pi^2$
5	$4M_\pi^2$	$4M_\pi^2$	$4(M_K^2+M_\pi^2)$
9	$2\tilde{Q}^2$	$2\tilde{Q}^2$	$2(s+t-u)-2(M_K^2-\tilde{Q}^2)$

and

$$\begin{aligned}
U_Z(s,t,u) &= s\Delta_0(s)+(t-u)\Delta_1(s)-\frac{4}{9}M_K^2M_\pi^2J_{\eta\eta}^r(s) \\
&+\frac{1}{32}\Big[+11(s-t+u)^2-20\left(M_K^2+M_\pi^2\right)(s-t+u) \\
&\qquad +12\left(M_K^2+M_\pi^2\right)^2\Big]J_{K\pi}^r(t) \\
&+\frac{1}{96}\left[3(s-t+u)-2\left(M_K^2+M_\pi^2\right)\right]^2J_{\eta K}^r(t) \\
&+\frac{1}{4}(s+t-u)^2J_{K\pi}^r(u) \\
&+\frac{1}{4}\left(M_K^2-M_\pi^2\right)\left[5(s-t+u)-6\left(M_K^2+M_\pi^2\right)\right]K_{K\pi}(t) \\
&+\frac{1}{4}\left(M_K^2-M_\pi^2\right)\left[3(s-t+u)-2\left(M_K^2+M_\pi^2\right)\right]K_{\eta K}(t) \\
&-\frac{3}{4}\left[3s+t-u-2\left(M_K^2+M_\pi^2\right)\right]\left[L_{K\pi}(t)+L_{\eta K}(t)\right] \\
&+\frac{3}{8}\Big\{+2s\left[t-u+4\left(M_K^2+M_\pi^2\right)\right] \\
&\qquad -3s^2+(t-u)^2-16M_K^2M_\pi^2\Big\}\left[M_{K\pi}^r(t)+M_{\eta K}^r(t)\right].
\end{aligned} \tag{4.35}$$

Once all terms C_X, $P_X(s,t,u)$, $U_X(s,t,u)$ have been inserted in Eq. (4.27) and the pole has been subtracted, one can determine the isospin components of $\mathcal{N}_{K^\pm}$, $\mathcal{H}_{K^\pm}$. The chiral representation can be obtained evaluating the isospin components (3.122) in the forward kinematics:

$$s=0 \qquad t=M_K^2+M_\pi^2-2M_K\nu \qquad u=M_K^2+M_\pi^2+2M_K\nu. \tag{4.36}$$

At tree level we find the results presented in Eq. (3.114).

Table 4.3: Coefficients $p_j^Z(s,t,u)$.

j	$p_j^Z(s,t,u)$
1	$32(s-2M_\pi^2)(s-2M_K^2)$
2	$8s^2+8(t-u)^2$
3	$-4(t-u)s-16(M_\pi^2+M_K^2)s+10s^2+2(t-u)^2+32M_K^2M_\pi^2$
4	$32(M_K^2+M_\pi^2)s-128M_K^2M_\pi^2$
5	$4(M_K^2+M_\pi^2)(s+t-u)-32M_K^2M_\pi^2$
6	$128M_K^2M_\pi^2$
8	$64M_K^2M_\pi^2$

Amplitude of Eta Meson

The amplitude entering the asymptotic formula for the mass of the eta meson is defined as

$$\mathcal{F}_\eta(\tilde{\nu},\vartheta_{\pi^+}) = T_{\eta\pi^0}(0,-4M_\eta\nu) + \left[T_{\eta\pi^+}(0,-4M_\eta\nu) + T_{\eta\pi^-}(0,-4M_\eta\nu)\right] \mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}. \tag{4.37}$$

The chiral representation can be determined from the $\eta\pi$-scattering,

$$\pi(p_1)+\eta(p_2)\longrightarrow\pi(p_3)+\eta(p_4), \tag{4.38}$$

in the forward kinematics. In ChPT the $\eta\pi$-scattering is given by the invariant amplitude $T_{\pi\eta}(s,t,u)$. The amplitude $T_{\pi\eta}(s,t,u)$ is invariant under the interchange of the first and the last arguments, i.e. $T_{\pi\eta}(s,t,u)=T_{\pi\eta}(u,t,s)$. This is a consequence of the fact that the eta meson is its own antiparticle: in the $\eta\pi$-scattering, we can interchange $p_2\leftrightarrow -p_4$ (i.e. $s\leftrightarrow u$) without changing the process. The isospin components of $\mathcal{F}_\eta$ can be all expressed in terms of $T_{\pi\eta}(s,t,u)$ in the same way,

$$\begin{aligned} T_{\eta\pi^0}(t,u-s) &= T_{\eta\pi^+}(t,u-s) \\ &= T_{\eta\pi^-}(t,u-s) \\ &= T_{\pi\eta}(s,t,u). \end{aligned} \tag{4.39}$$

The invariant amplitude is known up to NLO in the chiral expansion and reads

$$
\begin{aligned}
T_{\pi\eta}(s,t,u) = \frac{M_\pi^2}{3F_\pi^2} + \frac{1}{F_\pi^4}\Bigg\{ & + \frac{2M_\pi^2}{3N}(M_K^2\ell_K - M_\pi^2\ell_\pi) + 8L_1^{\mathrm{r}}(t-2M_\eta^2)(t-2M_\pi^2) \\
& + 4L_2^{\mathrm{r}}\Big[+ s^2 + u^2 + 2(M_\eta^2 + M_\pi^2) - 2M_\pi^2(s+u) \\
& \qquad - 2M_\eta^2(s+u-2M_\pi^2)\Big] \\
& + \frac{4}{3}L_3^{\mathrm{r}}\Big[+ s^2 + u^2 + t^2 + 2(M_\eta^2 + M_\pi^2) \\
& \qquad - 2M_\pi^2(s+t+u) - 2M_\eta^2(s+t+u-4M_\pi^2)\Big] \\
& + 8L_4^{\mathrm{r}}\Big[\left(M_\eta^2 + M_\pi^2\right) t - 4M_\eta^2 M_\pi^2\Big] \\
& - \frac{8}{3}M_\pi^2\Big[2L_5^{\mathrm{r}}M_\eta^2 - L_6^{\mathrm{r}}\left(15M_\eta^2 - 4M_K^2 + M_\pi^2\right)\Big] \\
& - 16M_\pi^2\Big[2L_7^{\mathrm{r}}\left(M_\eta^2 - M_\pi^2\right) - L_8^{\mathrm{r}}M_\pi^2\Big] \\
& + \frac{M_\pi^2}{6}\left(2t - M_\pi^2\right) J_{\pi\pi}^r(t) \\
& + \frac{1}{24}\left(3s - 3M_\eta^2 - M_\pi^2\right)^2 J_{KK}^r(s) \\
& + \frac{1}{24}\left(3u - 3M_\eta^2 - M_\pi^2\right)^2 J_{KK}^r(u) \\
& + \frac{1}{24}t\left(9t - 6M_\eta^2 - 2M_\pi^2\right) J_{KK}^r(t) \\
& + \frac{M_\pi^2}{18}\Big[2M_\pi^2\left[J_{\eta\pi}^r(s) + J_{\eta\pi}^r(u)\right] + (4M_\eta^2 - M_\pi^2)J_{\eta\pi}^r(u)\Big]\Bigg\},
\end{aligned}
\tag{4.40}
$$

see Ref. [46]. Here, $N = (4\pi)$, $\ell_P = 2\log(M_P/\mu)$ for $P = \pi, K, \eta$ and μ is the renormalization constant. The renormalized LEC L_j^{r} were introduced in Eq. (1.59) and the loop-integral function $J_{PQ}^r(t)$ is the defined for $P, Q = \pi, K, \eta$ in Eq. (4.21). The chiral representation of $\mathcal{F}_\eta$ can be obtained inserting the expression at NLO of $T_{\pi\eta}(s,t,u)$ in the isospin components (4.39) and evaluating in the forward kinematics:

$$
s = M_\eta^2 + M_\pi^2 + 2M_\eta\nu \qquad t = 0 \qquad u = M_\eta^2 + M_\pi^2 - 2M_\eta\nu. \tag{4.41}
$$

At tree level we find the result presented in Eq. (3.91).

4.1.2 Chiral Expansion

Having determined the chiral representation of the amplitudes, we now apply the asymptotic formulae derived in Chapter 3. The results are presented in Sections 4.2—4.4 where we relegate cumbersome expressions in Appendix D. To better organize the results we follow Ref. [32] and make use of the chiral expansion. Hereafter, we quickly explain how the asymptotic formulae are expanded and how the results are organized.

We keep the discussion general and consider a pseudoscalar meson P with the mass M_P and the twisting angle ϑ_P^μ. The amplitudes of Tab. 4.1 can be expressed in the generic forms,

$$\begin{aligned}\mathcal{X}_P(\tilde{\nu},\vartheta_{\pi^+}) &= Z_{P\pi^0}(0,-4M_P\nu) + \left[Z_{P\pi^+}(0,-4M_P\nu) + Z_{P\pi^-}(0,-4M_P\nu)\right]\mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}\\ \mathcal{Y}_P(\tilde{\nu},\vartheta_{\pi^+}) &= \left[Z_{P\pi^+}(0,-4M_P\nu) - Z_{P\pi^-}(0,-4M_P\nu)\right]\mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}},\end{aligned} \tag{4.42}$$

where $\nu = (s-u)/(4M_P)$ and $\tilde{\nu} = \nu/M_\pi$. The functions $Z_{P\pi^0}(t,u-s)$, $Z_{P\pi^+}(t,u-s)$, $Z_{P\pi^-}(t,u-s)$ are isospin components in infinite volume. We can imagine that the amplitude $\mathcal{X}_P(\tilde{\nu},\vartheta_{\pi^+})$ enters in the asymptotic formula for the observable X_P and estimates the corrections δX_P. Then, the resummed formula has the form

$$\begin{aligned}\delta X_P &= R(X_P) + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}})\\ R(X_P) &= \frac{1}{(4\pi)^2\lambda_P}\frac{M_\pi}{X_P}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\int_{\mathbb{R}}\frac{\mathrm{d}y}{|\vec{n}|}\,\mathrm{e}^{-\lambda_\pi|\vec{n}|\sqrt{1+y^2}}\left(1+y\frac{D_P}{M_P}\frac{\partial}{\partial y}\right)\mathcal{X}_P(iy,\vartheta_{\pi^+}),\end{aligned} \tag{4.43a}$$

where $\lambda_P = M_P L$, $D_P = \sqrt{M_P^2 + |\vec{\vartheta}_P|^2} - M_P$ and $\bar{\lambda} = \bar{M}L$ with $\bar{M} = (\sqrt{3}+1)M_\pi/\sqrt{2}$. Analogously, the amplitude $\mathcal{Y}_P(\tilde{\nu},\vartheta_{\pi^+})$ enters in the asymptotic formula for the renormalization term $\Delta\vartheta^\mu_{\mathscr{X}_P}$ estimating the spatial components:

$$\begin{aligned}\Delta\vec{\vartheta}_{\mathscr{X}_P} &= \vec{R}(\vartheta_{\mathscr{X}_P}) + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}})\\ \vec{R}(\vartheta_{\mathscr{X}_P}) &= -\frac{1}{2\,(4\pi)^2}\frac{M_\pi^2}{X_P}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\frac{\vec{n}}{|\vec{n}|}\int_{\mathbb{R}}\mathrm{d}y\;\mathrm{e}^{-\lambda_\pi|\vec{n}|\sqrt{1+y^2}}\,y\,\mathcal{Y}_P(iy,\vartheta_{\pi^+}).\end{aligned} \tag{4.43b}$$

For convenience, we decompose the two amplitudes as

$$\begin{aligned}\mathcal{X}_P(\tilde{\nu},\vartheta_{\pi^+}) &= \mathcal{X}_P(X_P,\pi^0) + \mathcal{X}_P(X_P,\pi^\pm)\,\mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}\\ \mathcal{Y}_P(\tilde{\nu},\vartheta_{\pi^+}) &= \mathcal{Y}_P(\vartheta_{\mathscr{X}_P})\,\mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}},\end{aligned} \tag{4.44}$$

and collect the isospin components in

$$\begin{aligned}\mathcal{X}_P(X_P,\pi^0) &= Z_{P\pi^0}(0,-4M_P\nu)\\ \mathcal{X}_P(X_P,\pi^\pm) &= Z_{P\pi^+}(0,-4M_P\nu) + Z_{P\pi^-}(0,-4M_P\nu)\\ \mathcal{Y}_P(\vartheta_{\mathscr{X}_P}) &= Z_{P\pi^+}(0,-4M_P\nu) - Z_{P\pi^-}(0,-4M_P\nu).\end{aligned} \tag{4.45}$$

In ChPT the amplitudes $\mathcal{X}_P(\tilde{\nu}, \vartheta_{\pi^+})$, $\mathcal{Y}_P(\tilde{\nu}, \vartheta_{\pi^+})$ can be developed according to the chiral expansion. The expansion is a series in powers of $\xi_P = M_P^2/(4\pi F_\pi)^2$ for which the amplitudes read

$$\begin{aligned}\mathcal{X}_P(\tilde{\nu}, \vartheta_{\pi^+}) &= \mathcal{X}_P^{(2)}(\tilde{\nu}, \vartheta_{\pi^+}) + \xi_P \mathcal{X}_P^{(4)}(\tilde{\nu}, \vartheta_{\pi^+}) + \mathcal{O}(\xi_P^2) \\ \mathcal{Y}_P(\tilde{\nu}, \vartheta_{\pi^+}) &= \mathcal{Y}_P^{(2)}(\tilde{\nu}, \vartheta_{\pi^+}) + \xi_P \mathcal{Y}_P^{(4)}(\tilde{\nu}, \vartheta_{\pi^+}) + \mathcal{O}(\xi_P^2).\end{aligned} \tag{4.46}$$

At each order the terms can be decomposed by means of Eq. (4.44) in

$$\begin{aligned}\mathcal{X}_P^{(j)}(\tilde{\nu}, \vartheta_{\pi^+}) &= \mathcal{X}_P^{(j)}(X_P, \pi^0) + \mathcal{X}_P^{(j)}(X_P, \pi^\pm) \mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}} \\ \mathcal{Y}_P^{(j)}(\tilde{\nu}, \vartheta_{\pi^+}) &= \mathcal{Y}_P^{(j)}(\vartheta_{\mathscr{X}_P}) \mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}},\end{aligned} \tag{4.47}$$

where $j = 2, 4, \ldots$ This decomposition allows us to factorize order by order the phase factor $\exp(iL\vec{n}\vec{\vartheta}_{\pi^+})$ within the chiral expansion (4.46). Then, the amplitudes can be expressed as

$$\begin{aligned}\mathcal{X}_P(\tilde{\nu}, \vartheta_{\pi^+}) = {} & \mathcal{X}_P^{(2)}(X_P, \pi^0) + \xi_P \mathcal{X}_P^{(4)}(X_P, \pi^0) + \mathcal{O}(\xi_P^2) \\ & + \left[\mathcal{X}_P^{(2)}(X_P, \pi^\pm) + \xi_P \mathcal{X}_P^{(2)}(X_P, \pi^\pm) + \mathcal{O}(\xi_P^2)\right] \mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}\end{aligned} \tag{4.48a}$$

$$\mathcal{Y}_P(\tilde{\nu}, \vartheta_{\pi^+}) = \left[\mathcal{Y}_P^{(2)}(\vartheta_{\mathscr{X}_P}) + \xi_P \mathcal{Y}_P^{(4)}(\vartheta_{\mathscr{X}_P}) + \mathcal{O}(\xi_P^2)\right] \mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}. \tag{4.48b}$$

These expressions induce a similar expansion in the asymptotic formulae. The asymptotic formula (4.43a) can be rewritten as

$$R(X_P) = R(X_P, \pi^0) + R(X_P, \pi^\pm) + R_D(X_P, \pi^0) + R_D(X_P, \pi^\pm), \tag{4.49}$$

with

$$\begin{aligned}R(X_P, \pi^0) &= \frac{\xi_\pi}{\lambda_\pi} \frac{X_\pi}{X_P} \sum_{\substack{\vec{n} \in \mathbb{Z}^3 \\ |\vec{n}| \neq 0}} \frac{1}{|\vec{n}|} \left[I^{(2)}(X_P, \pi^0) + \xi_P I^{(4)}(X_P, \pi^0) + \mathcal{O}(\xi_P^2)\right] \\ R(X_P, \pi^\pm) &= \frac{\xi_\pi}{\lambda_\pi} \frac{X_\pi}{X_P} \sum_{\substack{\vec{n} \in \mathbb{Z}^3 \\ |\vec{n}| \neq 0}} \frac{1}{|\vec{n}|} \left[I^{(2)}(X_P, \pi^\pm) + \xi_P I^{(4)}(X_P, \pi^\pm) + \mathcal{O}(\xi_P^2)\right] \mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}} \\ R_D(X_P, \pi^0) &= \frac{\xi_\pi}{\lambda_\pi} \frac{X_\pi}{X_P} \frac{D_P}{M_P} \sum_{\substack{\vec{n} \in \mathbb{Z}^3 \\ |\vec{n}| \neq 0}} \frac{1}{|\vec{n}|} \left[I_D^{(2)}(X_P, \pi^0) + \xi_P I_D^{(4)}(X_P, \pi^0) + \mathcal{O}(\xi_P^2)\right] \\ R_D(X_P, \pi^\pm) &= \frac{\xi_\pi}{\lambda_\pi} \frac{X_\pi}{X_P} \frac{D_P}{M_P} \sum_{\substack{\vec{n} \in \mathbb{Z}^3 \\ |\vec{n}| \neq 0}} \frac{1}{|\vec{n}|} \left[I_D^{(2)}(X_P, \pi^\pm) + \xi_P I_D^{(4)}(X_P, \pi^\pm) + \mathcal{O}(\xi_P^2)\right] \mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}.\end{aligned} \tag{4.50}$$

The contributions $R(X_P, \pi^0)$, $R_D(X_P, \pi^0)$ originate from $\mathcal{X}_P(X_P, \pi^0)$ and hence, from the virtual neutral pion. The contributions $R(X_P, \pi^\pm)$, $R_D(X_P, \pi^\pm)$ originate from $\mathcal{X}_P(X_P, \pi^\pm)$

and hence, from virtual charged pions. Here, all contributions are rescaled by X_π/X_P where X_π is the observable X_P in infinite volume for $P=\pi$. Note that $R_D(X_P,\pi^0)$, $R_D(X_P,\pi^\pm)$ are proportional to the parameter D_P and disappear if $\vartheta^\mu_P=0$. The contributions involve integrals $I^{(j)}(X_P,\pi^0)$, ..., $I^{(j)}_D(X_P,\pi^\pm)$ which can be determined from the terms $\mathcal{X}^{(j)}_P(X_P,\pi^0)$, $\mathcal{X}^{(j)}_P(X_P,\pi^\pm)$ of the decomposition (4.47).

The expression (4.48b) induces a similar expansion in the asymptotic formula (4.43b). The formula can be rewritten as

$$\vec{R}(\vartheta_{\mathscr{X}_P}) = -\frac{\xi_\pi M_P}{2}\frac{X_\pi}{X_P}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\frac{i\vec{n}}{|\vec{n}|}\left[I^{(2)}(\vartheta_{\mathscr{X}_P})+\xi_P I^{(4)}(\vartheta_{\mathscr{X}_P})+\mathcal{O}(\xi_P^2)\right]\mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}. \tag{4.51}$$

This formula just contains contributions originating from virtual charged pions. The integrals $I^{(j)}(\vartheta_{\mathscr{X}_P})$ can be determined from the term $\mathcal{Y}^{(j)}_P(\vartheta_{\mathscr{X}_P})$ of the decomposition (4.47). Note that $\vec{R}(\vartheta_{\mathscr{X}_P})$ is absent if the particle P has no twisting angle, namely if $\vartheta^\mu_P=0$. Moreover, $\vec{R}(\vartheta_{\mathscr{X}_P})$ disappears for $\vartheta^\mu_{\pi^+}=0$ due to the odd sum in $\vec{n}$.

In the following we present the results obtained applying the asymptotic formulae of Chapter 3. We expand the asymptotic formulae as in Eqs. (4.49, 4.51) and write down the expressions of their integrals. The integrals can be in large part evaluated analytically but in some case they must be estimated numerically. We present their expressions up to NLO separating the part evaluated analytically from terms estimated numerically.

4.2 Asymptotic Formulae for Pions

4.2.1 Masses

We start with the asymptotic formulae for pion masses. The formula of the neutral pion reads

$$\begin{aligned}\delta M_{\pi^0} &= R(M_{\pi^0})+\mathcal{O}(\mathrm{e}^{-\bar{\lambda}})\\ R(M_{\pi^0}) &= -\frac{1}{2\,(4\pi)^2\,\lambda_\pi}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\int_{\mathbb{R}}\frac{\mathrm{d}y}{|\vec{n}|}\,e^{-\lambda_\pi|\vec{n}|\sqrt{1+y^2}}\,\mathcal{F}_{\pi^0}(iy,\vartheta_{\pi^+}).\end{aligned} \tag{4.52}$$

We insert the chiral representation of $\mathcal{F}_{\pi^0}$ obtained from the isospin components (4.4) and expand the representation according to Eq. (4.48a). The asymptotic formula exhibits two contributions

$$R(M_{\pi^0}) = R(M_{\pi^0},\pi^0)+R(M_{\pi^0},\pi^\pm), \tag{4.53}$$

with

$$\begin{aligned}R(M_{\pi^0},\pi^0) &= -\frac{\xi_\pi}{2\lambda_\pi}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\frac{1}{|\vec{n}|}\left[I^{(2)}(M_{\pi^0},\pi^0)+\xi_\pi I^{(4)}(M_{\pi^0},\pi^0)\right]\\ R(M_{\pi^0},\pi^\pm) &= -\frac{\xi_\pi}{2\lambda_\pi}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\frac{1}{|\vec{n}|}\left[I^{(2)}(M_{\pi^0},\pi^\pm)+\xi_\pi I^{(4)}(M_{\pi^0},\pi^\pm)\right]\mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}.\end{aligned} \tag{4.54}$$

The integrals $I^{(2)}(M_{\pi^0},\pi^0)$, $I^{(4)}(M_{\pi^0},\pi^0)$ resp. $I^{(2)}(M_{\pi^0},\pi^\pm)$, $I^{(4)}(M_{\pi^0},\pi^\pm)$ were first calculated in the framework of twisted mass ChPT in Ref. [26]. Here, we consider ordinary ChPT and find

$$I^{(2)}(M_{\pi^0},\pi^0) = B^0 \tag{4.55a}$$

$$I^{(2)}(M_{\pi^0},\pi^\pm) = -2\,B^0 \tag{4.55b}$$

$$\begin{aligned} I^{(4)}(M_{\pi^0},\pi^0) &= -B^0\left[\frac{9}{2}-\frac{4}{3}\bar\ell_1-\frac{8}{3}\bar\ell_2+\frac{3}{2}\bar\ell_3-2\bar\ell_4\right]+B^2\left[8-\frac{8}{3}\bar\ell_1-\frac{16}{3}\bar\ell_2\right] \\ &\quad + S^{(4)}(M_{\pi^0},\pi^0) \qquad (4.55\mathrm{c}) \\ I^{(4)}(M_{\pi^0},\pi^\pm) &= B^0\left[\frac{13}{9}+\frac{8}{3}\bar\ell_1-\bar\ell_3-4\bar\ell_4\right]+B^2\left[\frac{40}{9}-\frac{16}{3}\bar\ell_2\right]+S^{(4)}(M_{\pi^0},\pi^\pm). \qquad (4.55\mathrm{d}) \end{aligned}$$

The above expressions are in accordance with the results of Ref. [26]. The functions $B^{2k}=B^{2k}(\lambda_\pi|\vec n|)$ were introduced in Ref. [25] and are evaluable analytically

$$\begin{aligned} B^{2k} &= \int_{\mathbb{R}} \mathrm{d}y\, y^{2k}\, \mathrm{e}^{-\lambda_\pi|\vec n|\sqrt{1+y^2}} \\ &= \frac{\Gamma(k+1/2)}{\Gamma(3/2)}\left[\frac{2}{\lambda_\pi|\vec n|}\right]^k K_{k+1}(\lambda_\pi|\vec n|). \end{aligned} \tag{4.56}$$

Here, $K_j(x)$ are modified Bessel functions of the second kind. The μ-independent constants $\bar\ell_j$ were introduced in Eq. (1.66). They depend logarithmically on the pion mass,

$$\bar\ell_j = \bar\ell_j^{\mathrm{phys}} + 2\log\left(\frac{M_\pi^{\mathrm{phys}}}{M_\pi}\right), \tag{4.57}$$

where $M_\pi^{\mathrm{phys}} = 0.140$ GeV is the physical value of Tab. 1.2 and $\bar\ell_j^{\mathrm{phys}}$ are listed in Tab. 5.1. The terms $S^{(4)}(M_{\pi^0},\pi^0)$, $S^{(4)}(M_{\pi^0},\pi^\pm)$ contain integrals that can not be evaluated analytically but just estimated numerically. In Eq. (D.1) we give their explicit expressions.

The asymptotic formulae for the masses of the charged pions read

$$\begin{aligned} \delta M_{\pi^\pm} &= R(M_{\pi^\pm}) + \mathcal{O}(\mathrm{e}^{-\bar\lambda}) \\ R(M_{\pi^\pm}) &= -\frac{1}{2\,(4\pi)^2\,\lambda_\pi}\sum_{\substack{\vec n\in\mathbb{Z}^3\\ |\vec n|\neq 0}}\int_{\mathbb{R}}\frac{\mathrm{d}y}{|\vec n|}\,\mathrm{e}^{-\lambda_\pi|\vec n|\sqrt{1+y^2}}\left(1+y\frac{D_{\pi^\pm}}{M_\pi}\frac{\partial}{\partial y}\right)\mathcal{F}_{\pi^\pm}(iy,\vartheta_{\pi^+}), \end{aligned} \tag{4.58}$$

where $D_{\pi^\pm} = \sqrt{M_\pi^2+|\vec\vartheta_{\pi^\pm}|^2}-M_\pi$. We insert the chiral representation of $\mathcal{F}_{\pi^\pm}$ obtained from the isospin components (4.4) and expand the representation according to Eq. (4.48a). The asymptotic formulae exhibit four contributions,

$$R(M_{\pi^\pm}) = R(M_{\pi^\pm},\pi^0)+R(M_{\pi^\pm},\pi^\pm)+R_D(M_{\pi^\pm},\pi^0)+R_D(M_{\pi^\pm},\pi^\pm), \tag{4.59}$$

where

$$
\begin{aligned}
R(M_{\pi^\pm},\pi^0) &= -\frac{\xi_\pi}{2\lambda_\pi}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\frac{1}{|\vec{n}|}\left[I^{(2)}(M_{\pi^\pm},\pi^0)+\xi_\pi I^{(4)}(M_{\pi^\pm},\pi^0)\right]\\
R(M_{\pi^\pm},\pi^\pm) &= -\frac{\xi_\pi}{2\lambda_\pi}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\frac{1}{|\vec{n}|}\left[I^{(2)}(M_{\pi^\pm},\pi^\pm)+\xi_\pi I^{(4)}(M_{\pi^\pm},\pi^\pm)\right]\mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}\\
R_D(M_{\pi^\pm},\pi^0) &= -\frac{\xi_\pi}{2\lambda_\pi}\frac{D_{\pi^\pm}}{M_\pi}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\frac{1}{|\vec{n}|}\left[I_D^{(2)}(M_{\pi^\pm},\pi^0)+\xi_\pi I_D^{(4)}(M_{\pi^\pm},\pi^0)\right]\\
R_D(M_{\pi^\pm},\pi^\pm) &= -\frac{\xi_\pi}{2\lambda_\pi}\frac{D_{\pi^\pm}}{M_\pi}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\frac{1}{|\vec{n}|}\left[I_D^{(2)}(M_{\pi^\pm},\pi^\pm)+\xi_\pi I_D^{(4)}(M_{\pi^\pm},\pi^\pm)\right]\mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}.
\end{aligned}
\tag{4.60}
$$

The integrals $I^{(2)}(M_{\pi^\pm},\pi^0)$, $I^{(4)}(M_{\pi^\pm},\pi^0)$ resp. $I^{(2)}(M_{\pi^\pm},\pi^\pm)$, $I^{(4)}(M_{\pi^\pm},\pi^\pm)$ were calculated in twisted mass ChPT, see Ref. [26]. In accordance with the results of Ref. [26], we find

$$I^{(2)}(M_{\pi^\pm},\pi^0) = -B^0 \tag{4.61a}$$

$$I^{(2)}(M_{\pi^\pm},\pi^\pm) = 0 \tag{4.61b}$$

$$I^{(4)}(M_{\pi^\pm},\pi^0) = B^0\left[\frac{13}{18}+\frac{4}{3}\bar{\ell}_1-\frac{1}{2}\bar{\ell}_3-2\bar{\ell}_4\right]+B^2\left[\frac{20}{9}-\frac{8}{3}\bar{\ell}_2\right]+S^{(4)}(M_{\pi^\pm},\pi^0) \tag{4.61c}$$

$$
\begin{aligned}
I^{(4)}(M_{\pi^\pm},\pi^\pm) = -B^0\left[\frac{34}{9}-\frac{8}{3}\bar{\ell}_1-\frac{8}{3}\bar{\ell}_2+2\bar{\ell}_3\right]+B^2\left[\frac{92}{9}-\frac{8}{3}\bar{\ell}_1-8\bar{\ell}_2\right]\\
+S^{(4)}(M_{\pi^\pm},\pi^\pm),
\end{aligned}
\tag{4.61d}
$$

where $S^{(4)}(M_{\pi^\pm},\pi^0)$, $S^{(4)}(M_{\pi^\pm},\pi^\pm)$ are given in Eq. (D.2). Note that these integrals are related to that ones of Eq. (4.55) by means of

$$
\begin{aligned}
I^{(j)}(M_{\pi^\pm},\pi^0) &= \frac{1}{2}\,I^{(j)}(M_{\pi^0},\pi^\pm)\\
I^{(j)}(M_{\pi^\pm},\pi^\pm) &= I^{(j)}(M_{\pi^0},\pi^0)+\frac{1}{2}\,I^{(j)}(M_{\pi^0},\pi^\pm),
\end{aligned}
\tag{4.62}
$$

where $j=2,4$. These identities follow from the relations between the isospin components of the neutral and charged pions, see Eq. (4.4).

The integrals $I_D^{(2)}(M_{\pi^\pm},\pi^0)$, $I_D^{(4)}(M_{\pi^\pm},\pi^0)$ resp. $I_D^{(2)}(M_{\pi^\pm},\pi^\pm)$, $I_D^{(4)}(M_{\pi^\pm},\pi^\pm)$ can be evaluated from the derivative $\partial_y \mathcal{F}_{\pi^\pm}$. We find

$$I_D^{(2)}(M_{\pi^\pm}, \pi^0) = I_D^{(2)}(M_{\pi^\pm}, \pi^\pm) = 0 \tag{4.63a}$$

$$I_D^{(4)}(M_{\pi^\pm}, \pi^0) = B^2 \left[\frac{40}{9} - \frac{16}{3}\bar{\ell}_2\right] + S_D^{(4)}(M_{\pi^\pm}, \pi^0) \tag{4.63b}$$

$$I_D^{(4)}(M_{\pi^\pm}, \pi^\pm) = B^2 \left[\frac{184}{9} - \frac{16}{3}\bar{\ell}_1 - 16\bar{\ell}_2\right] + S_D^{(4)}(M_{\pi^\pm}, \pi^\pm), \tag{4.63c}$$

where $S_D^{(4)}(M_{\pi^\pm}, \pi^0)$, $S_D^{(4)}(M_{\pi^\pm}, \pi^\pm)$ are given in Eq. (D.3).

The asymptotic formulae for the renormalization terms $\Delta\vartheta^\mu_{\Sigma_{\pi^\pm}}$ read

$$\begin{aligned} \Delta\vec{\vartheta}_{\Sigma_{\pi^\pm}} &= \vec{R}(\vartheta_{\Sigma_{\pi^\pm}}) + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}}) \\ \vec{R}(\vartheta_{\Sigma_{\pi^\pm}}) &= -\frac{M_\pi}{2\,(4\pi)^2} \sum_{\substack{\vec{n}\in\mathbb{Z}^3 \\ |\vec{n}|\neq 0}} \frac{\vec{n}}{|\vec{n}|} \int_{\mathbb{R}} \mathrm{d}y\ \mathrm{e}^{-\lambda_\pi |\vec{n}|\sqrt{1+y^2}}\ y\ \mathcal{G}_{\pi^\pm}(iy, \vartheta_{\pi^+}). \end{aligned} \tag{4.64}$$

We insert the chiral representation of $\mathcal{G}_{\pi^\pm}$ obtained from the isospin components (4.4) and expand the representation according to Eq. (4.48b). The asymptotic formulae can be written as

$$\vec{R}(\vartheta_{\Sigma_{\pi^\pm}}) = -\frac{\xi_\pi M_\pi}{2} \sum_{\substack{\vec{n}\in\mathbb{Z}^3 \\ |\vec{n}|\neq 0}} \frac{i\vec{n}}{|\vec{n}|} \left[I^{(2)}(\vartheta_{\Sigma_{\pi^\pm}}) + \xi_\pi I^{(4)}(\vartheta_{\Sigma_{\pi^\pm}})\right] \mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}. \tag{4.65}$$

The integrals can be evaluated from the chiral representation of $\mathcal{G}_{\pi^\pm}$. We find

$$I^{(2)}(\vartheta_{\Sigma_{\pi^\pm}}) = \pm\left\{-4B^2\right\} \tag{4.66a}$$

$$I^{(4)}(\vartheta_{\Sigma_{\pi^\pm}}) = \pm\left\{8B^2\left[1 - \bar{\ell}_4\right] + S^{(4)}(\vartheta_{\Sigma_{\pi^+}})\right\}, \tag{4.66b}$$

where $S^{(4)}(\vartheta_{\Sigma_{\pi^+}})$ is given in Eq. (D.4).

4.2.2 Decay Constants

The asymptotic formula for the decay constant of the neutral pion reads

$$\begin{aligned} \delta F_{\pi^0} &= R(F_{\pi^0}) + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}}) \\ R(F_{\pi^0}) &= \frac{1}{(4\pi)^2\,\lambda_\pi} \frac{M_\pi}{F_\pi} \sum_{\substack{\vec{n}\in\mathbb{Z}^3 \\ |\vec{n}|\neq 0}} \int_{\mathbb{R}} \frac{\mathrm{d}y}{|\vec{n}|}\ \mathrm{e}^{-\lambda_\pi |\vec{n}|\sqrt{1+y^2}}\, \mathcal{N}_{\pi^0}(iy, \vartheta_{\pi^+}). \end{aligned} \tag{4.67}$$

In Section 3.4.2 we have seen that $\mathcal{N}_{\pi^0}$ is related to $\mathcal{F}_{\pi^0}$, $\mathcal{C}_{\pi^0}$ by virtue of Eq. (3.156). We use this relation to determine the chiral representation of $\mathcal{N}_{\pi^0}$ at one loop. If we insert the chiral representation in the asymptotic formula and expand according to Eq. (4.48a), we obtain

$$R(F_{\pi^0}) = R(F_{\pi^0},\pi^0) + R(F_{\pi^0},\pi^\pm), \tag{4.68}$$

with

$$\begin{aligned} R(F_{\pi^0},\pi^0) &= \frac{\xi_\pi}{\lambda_\pi}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\frac{1}{|\vec{n}|}\left[I^{(2)}(F_{\pi^0},\pi^0)+\xi_\pi I^{(4)}(F_{\pi^0},\pi^0)\right]\\ R(F_{\pi^0},\pi^\pm) &= \frac{\xi_\pi}{\lambda_\pi}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\frac{1}{|\vec{n}|}\left[I^{(2)}(F_{\pi^0},\pi^\pm)+\xi_\pi I^{(4)}(F_{\pi^0},\pi^\pm)\right]\mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}. \end{aligned} \tag{4.69}$$

The integrals $I^{(2)}(F_{\pi^0},\pi^0)$, $I^{(4)}(F_{\pi^0},\pi^0)$ resp. $I^{(2)}(F_{\pi^0},\pi^\pm)$, $I^{(4)}(F_{\pi^0},\pi^\pm)$ are related to those of Eqs. (4.55, 4.82) and value

$$I^{(2)}(F_{\pi^0},\pi^0) = 0 \tag{4.70a}$$

$$I^{(2)}(F_{\pi^0},\pi^\pm) = -2\,B^0 \tag{4.70b}$$

$$I^{(4)}(F_{\pi^0},\pi^0) = -B^0\left[1-\frac{2}{3}\bar{\ell}_1-\frac{4}{3}\bar{\ell}_2+\bar{\ell}_4\right]+B^2\left[8-\frac{8}{3}\bar{\ell}_1-\frac{16}{3}\bar{\ell}_2\right]+S^{(4)}(F_{\pi^0},\pi^0) \tag{4.70c}$$

$$I^{(4)}(F_{\pi^0},\pi^\pm) = B^0\left[\frac{2}{9}+\frac{4}{3}\bar{\ell}_1-2\bar{\ell}_4\right]+B^2\left[\frac{40}{9}-\frac{16}{3}\bar{\ell}_2\right]+S^{(4)}(F_{\pi^0},\pi^\pm). \tag{4.70d}$$

The terms $S^{(4)}(F_{\pi^0},\pi^0)$, $S^{(4)}(F_{\pi^0},\pi^\pm)$ are explicitly given in Eq. (D.5).

The asymptotic formulae for the decay constants of charged pions read

$$\begin{aligned} \delta F_{\pi^\pm} &= R(F_{\pi^\pm}) + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}})\\ R(F_{\pi^\pm}) &= \frac{1}{(4\pi)^2\,\lambda_\pi}\frac{M_\pi}{F_\pi}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\int_{\mathbb{R}}\frac{\mathrm{d}y}{|\vec{n}|}\,\mathrm{e}^{-\lambda_\pi|\vec{n}|\sqrt{1+y^2}}\left(1+y\frac{D_{\pi^\pm}}{M_\pi}\frac{\partial}{\partial y}\right)\mathcal{N}_{\pi^\pm}(iy,\vartheta_{\pi^+}), \end{aligned} \tag{4.71}$$

where $D_{\pi^\pm}$ are the parameters given in Eq. (3.57). We insert the chiral representation of $\mathcal{N}_{\pi^\pm}$ obtained from the isospin components (3.111) and expand according to Eq. (4.48a). The asymptotic formulae exhibit four contributions

$$R(F_{\pi^\pm}) = R(F_{\pi^\pm},\pi^0) + R(F_{\pi^\pm},\pi^\pm) + R_D(F_{\pi^\pm},\pi^0) + R_D(F_{\pi^\pm},\pi^\pm), \tag{4.72}$$

where

$$\begin{aligned}
R(F_{\pi^\pm},\pi^0) &= \frac{\xi_\pi}{\lambda_\pi}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\frac{1}{|\vec{n}|}\left[I^{(2)}(F_{\pi^\pm},\pi^0)+\xi_\pi I^{(4)}(F_{\pi^\pm},\pi^0)\right]\\
R(F_{\pi^\pm},\pi^\pm) &= \frac{\xi_\pi}{\lambda_\pi}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\frac{1}{|\vec{n}|}\left[I^{(2)}(F_{\pi^\pm},\pi^\pm)+\xi_\pi I^{(4)}(F_{\pi^\pm},\pi^\pm)\right]\mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}\\
R_D(F_{\pi^\pm},\pi^0) &= \frac{\xi_\pi}{\lambda_\pi}\frac{D_{\pi^\pm}}{M_\pi}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\frac{1}{|\vec{n}|}\left[I_D^{(2)}(F_{\pi^\pm},\pi^0)+\xi_\pi I_D^{(4)}(F_{\pi^\pm},\pi^0)\right]\\
R_D(F_{\pi^\pm},\pi^\pm) &= \frac{\xi_\pi}{\lambda_\pi}\frac{D_{\pi^\pm}}{M_\pi}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\frac{1}{|\vec{n}|}\left[I_D^{(2)}(F_{\pi^\pm},\pi^\pm)+\xi_\pi I_D^{(4)}(F_{\pi^\pm},\pi^\pm)\right]\mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}.
\end{aligned}\tag{4.73}$$

The integrals $I^{(2)}(F_{\pi^\pm},\pi^0)$, $I^{(4)}(F_{\pi^\pm},\pi^0)$ resp. $I^{(2)}(F_{\pi^\pm},\pi^\pm)$, $I^{(4)}(F_{\pi^\pm},\pi^\pm)$ were calculated in twisted mass ChPT, see Ref. [26]. In accordance with the results of Ref. [26], we find

$$I^{(2)}(F_{\pi^\pm},\pi^0) = I^{(2)}(F_{\pi^\pm},\pi^\pm) = -B^0 \tag{4.74a}$$

$$I^{(4)}(F_{\pi^\pm},\pi^0) = B^0\left[\frac{1}{9}+\frac{2}{3}\bar{\ell}_1-\bar{\ell}_4\right]+B^2\left[\frac{20}{9}-\frac{8}{3}\bar{\ell}_2\right]+S^{(4)}(F_{\pi^\pm},\pi^0) \tag{4.74b}$$

$$\begin{aligned}I^{(4)}(F_{\pi^\pm},\pi^\pm) = -B^0\left[\frac{8}{9}-\frac{4}{3}\bar{\ell}_1-\frac{4}{3}\bar{\ell}_2+2\bar{\ell}_4\right]+B^2\left[\frac{92}{9}-\frac{8}{3}\bar{\ell}_1-8\bar{\ell}_2\right]&\\
+S^{(4)}(F_{\pi^\pm},\pi^\pm).&\end{aligned} \tag{4.74c}$$

The terms $S^{(4)}(F_{\pi^\pm},\pi^0)$, $S^{(4)}(F_{\pi^\pm},\pi^\pm)$ are given in Eq. (D.6).

The integrals $I_D^{(2)}(F_{\pi^\pm},\pi^0)$, $I_D^{(2)}(F_{\pi^\pm},\pi^0)$ resp. $I_D^{(2)}(F_{\pi^\pm},\pi^\pm)$, $I_D^{(4)}(F_{\pi^\pm},\pi^\pm)$ can be evaluated from the derivative $\partial_y\mathcal{N}_{\pi^\pm}$. We find

$$I_D^{(2)}(F_{\pi^\pm},\pi^0) = I_D^{(2)}(F_{\pi^\pm},\pi^\pm) = 0 \tag{4.75a}$$

$$I_D^{(4)}(F_{\pi^\pm},\pi^0) = B^2\left[\frac{40}{9}-\frac{16}{3}\bar{\ell}_2\right]+S_D^{(4)}(F_{\pi^\pm},\pi^0) \tag{4.75b}$$

$$I_D^{(4)}(F_{\pi^\pm},\pi^\pm) = B^2\left[\frac{184}{9}-\frac{16}{3}\bar{\ell}_1-16\bar{\ell}_2\right]+S_D^{(4)}(F_{\pi^\pm},\pi^\pm), \tag{4.75c}$$

where $S_D^{(4)}(F_{\pi^\pm},\pi^0)$, $S_D^{(4)}(F_{\pi^\pm},\pi^\pm)$ are given in Eq. (D.7).

The asymptotic formulae for the renormalization terms $\Delta\vartheta^{\mu}_{\mathscr{A}_{\pi^\pm}}$ read

$$\begin{aligned}\Delta\vec{\vartheta}_{\mathscr{A}_{\pi^\pm}} &= \vec{R}(\vartheta_{\mathscr{A}_{\pi^\pm}}) + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}}) \\ \vec{R}(\vartheta_{\mathscr{A}_{\pi^\pm}}) &= -\frac{1}{2\,(4\pi)^2}\frac{M_\pi^2}{F_\pi}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\frac{\vec{n}}{|\vec{n}|}\int_{\mathbb{R}}\mathrm{d}y\;\mathrm{e}^{-\lambda_\pi|\vec{n}|\sqrt{1+y^2}}\;y\;\mathcal{H}_{\pi^\pm}(iy,\vartheta_{\pi^+}).\end{aligned} \tag{4.76}$$

We insert the chiral representation of $\mathcal{H}_{\pi^\pm}$ obtained from the isospin components (3.111) and expand according to Eq. (4.48b). The asymptotic formulae can be written as

$$\vec{R}(\vartheta_{\mathscr{A}_{\pi^\pm}}) = -\frac{\xi_\pi M_\pi}{2}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\frac{i\vec{n}}{|\vec{n}|}\left[I^{(2)}(\vartheta_{\mathscr{A}_{\pi^\pm}}) + \xi_\pi I^{(4)}(\vartheta_{\mathscr{A}_{\pi^\pm}})\right]\mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}. \tag{4.77}$$

The integrals can be evaluated from the chiral representation of $\mathcal{H}_{\pi^\pm}$. We find

$$I^{(2)}(\vartheta_{\mathscr{A}_{\pi^\pm}}) = \pm\left\{-4B^2\right\} \tag{4.78a}$$

$$I^{(4)}(\vartheta_{\mathscr{A}_{\pi^\pm}}) = \pm\left\{4B^2\left[1-\bar{\ell}_4\right] + S^{(4)}(\vartheta_{\mathscr{A}_{\pi^+}})\right\}, \tag{4.78b}$$

where $S^{(4)}(\vartheta_{\mathscr{A}_{\pi^+}})$ is given in Eq. (D.8).

4.2.3 Pseudoscalar Coupling Constants

The asymptotic formula for the pseudoscalar coupling constant of the neutral pion reads

$$\begin{aligned}\delta G_{\pi^0} &= R(G_{\pi^0}) + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}}) \\ R(G_{\pi^0}) &= \frac{1}{(4\pi)^2\,\lambda_\pi}\frac{M_\pi^2}{G_\pi}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\int_{\mathbb{R}}\frac{\mathrm{d}y}{|\vec{n}|}\;\mathrm{e}^{-\lambda_\pi|\vec{n}|\sqrt{1+y^2}}\,\mathcal{C}_{\pi^0}(iy,\vartheta_{\pi^+}).\end{aligned} \tag{4.79}$$

We insert the chiral representation of $\mathcal{C}_{\pi^0}$ obtained subtracting the pole from Eq. (4.12) and expand according to Eq. (4.48a). The asymptotic formula exhibits two contributions,

$$R(G_{\pi^0}) = R(G_{\pi^0},\pi^0) + R(G_{\pi^0},\pi^\pm), \tag{4.80}$$

with

$$\begin{aligned}R(G_{\pi^0},\pi^0) &= \frac{\xi_\pi}{\lambda_\pi}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\frac{1}{|\vec{n}|}\left[I^{(2)}(G_{\pi^0},\pi^0) + \xi_\pi I^{(4)}(G_{\pi^0},\pi^0)\right] \\ R(G_{\pi^0},\pi^\pm) &= \frac{\xi_\pi}{\lambda_\pi}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\frac{1}{|\vec{n}|}\left[I^{(2)}(G_{\pi^0},\pi^\pm) + \xi_\pi I^{(4)}(G_{\pi^0},\pi^\pm)\right]\mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}.\end{aligned} \tag{4.81}$$

The integrals $I^{(2)}(G_{\pi^0},\pi^0)$, $I^{(4)}(G_{\pi^0},\pi^0)$ resp. $I^{(2)}(G_{\pi^0},\pi^\pm)$, $I^{(4)}(G_{\pi^0},\pi^\pm)$ can be evaluated from the chiral representation of $\mathcal{C}_{\pi^0}$. We find

$$I^{(2)}(G_{\pi^0},\pi^0) = -B^0 \tag{4.82a}$$

$$I^{(2)}(G_{\pi^0},\pi^\pm) = 0 \tag{4.82b}$$

$$I^{(4)}(G_{\pi^0},\pi^0) = B^0\left[\frac{7}{2}-\frac{2}{3}\bar{\ell}_1-\frac{4}{3}\bar{\ell}_2+\frac{3}{2}\bar{\ell}_3-3\bar{\ell}_4\right]+S^{(4)}(G_{\pi^0},\pi^0) \tag{4.82c}$$

$$I^{(4)}(G_{\pi^0},\pi^\pm) = -B^0\left[\frac{11}{9}+\frac{4}{3}\bar{\ell}_1-\bar{\ell}_3-2\bar{\ell}_4\right]+S^{(4)}(G_{\pi^0},\pi^\pm). \tag{4.82d}$$

The terms $S^{(4)}(G_{\pi^0},\pi^0)$, $S^{(4)}(G_{\pi^0},\pi^\pm)$ are explicitly given in Eq. (D.9). Note that by virtue of Eq. (3.151) these integrals are related to those of the mass and of the decay constant through

$$\begin{aligned} I^{(j)}(G_{\pi^0},\pi^0) &= I^{(j)}(F_{\pi^0},\pi^0) - I^{(j)}(M_{\pi^0},\pi^0)\\ I^{(j)}(G_{\pi^0},\pi^\pm) &= I^{(j)}(F_{\pi^0},\pi^\pm) - I^{(j)}(M_{\pi^0},\pi^\pm), \end{aligned} \tag{4.83}$$

where $j=2,4$. These relations follow from chiral Ward identities and allow us to evaluate the integrals of Eq. (4.70).

The asymptotic formulae for the pseudoscalar coupling constants of charged pions read

$$\begin{aligned} \delta G_{\pi^\pm} &= R(G_{\pi^\pm}) + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}})\\ R(G_{\pi^\pm}) &= \frac{1}{(4\pi)^2\lambda_\pi}\frac{M_\pi^2}{G_\pi}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\ |\vec{n}|\neq 0}}\int_{\mathbb{R}}\frac{\mathrm{d}y}{|\vec{n}|}\,\mathrm{e}^{-\lambda_\pi|\vec{n}|\sqrt{1+y^2}}\left(1+y\frac{D_{\pi^\pm}}{M_\pi}\frac{\partial}{\partial y}\right)\mathcal{C}_{\pi^\pm}(iy,\vartheta_{\pi^+}). \end{aligned} \tag{4.84}$$

We insert the chiral representation of $\mathcal{C}_{\pi^\pm}$ obtained from the isospin components (3.131) and expand according to Eq. (4.48a). The asymptotic formulae exhibit four contributions,

$$R(G_{\pi^\pm}) = R(G_{\pi^\pm},\pi^0) + R(G_{\pi^\pm},\pi^\pm) + R_D(G_{\pi^\pm},\pi^0) + R_D(G_{\pi^\pm},\pi^\pm), \tag{4.85}$$

with

$$
\begin{aligned}
R(G_{\pi^\pm},\pi^0) &= \frac{\xi_\pi}{\lambda_\pi}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\frac{1}{|\vec{n}|}\left[I^{(2)}(G_{\pi^\pm},\pi^0)+\xi_\pi I^{(4)}(G_{\pi^\pm},\pi^0)\right]\\
R(G_{\pi^\pm},\pi^\pm) &= \frac{\xi_\pi}{\lambda_\pi}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\frac{1}{|\vec{n}|}\left[I^{(2)}(G_{\pi^\pm},\pi^\pm)+\xi_\pi I^{(4)}(G_{\pi^\pm},\pi^\pm)\right]\mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}\\
R_D(G_{\pi^\pm},\pi^0) &= \frac{\xi_\pi}{\lambda_\pi}\frac{D_{\pi^\pm}}{M_\pi}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\frac{1}{|\vec{n}|}\left[I_D^{(2)}(G_{\pi^\pm},\pi^0)+\xi_\pi I_D^{(4)}(G_{\pi^\pm},\pi^0)\right]\\
R_D(G_{\pi^\pm},\pi^\pm) &= \frac{\xi_\pi}{\lambda_\pi}\frac{D_{\pi^\pm}}{M_\pi}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\frac{1}{|\vec{n}|}\left[I_D^{(2)}(G_{\pi^\pm},\pi^\pm)+\xi_\pi I_D^{(4)}(G_{\pi^\pm},\pi^\pm)\right]\mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}.
\end{aligned}
\tag{4.86}
$$

The integrals $I^{(2)}(G_{\pi^\pm},\pi^0)$, $I^{(4)}(G_{\pi^\pm},\pi^0)$ resp. $I^{(2)}(G_{\pi^\pm},\pi^\pm)$, $I^{(4)}(G_{\pi^\pm},\pi^\pm)$ can be evaluated from the chiral representation of $\mathcal{C}_{\pi^\pm}$. We find

$$I^{(2)}(G_{\pi^\pm},\pi^0) = 0 \tag{4.87a}$$

$$I^{(2)}(G_{\pi^\pm},\pi^\pm) = -B^0 \tag{4.87b}$$

$$I^{(4)}(G_{\pi^\pm},\pi^0) = -B^0\left[\frac{11}{18}+\frac{2}{3}\bar{\ell}_1-\frac{\bar{\ell}_3}{2}-\bar{\ell}_4\right]+S^{(4)}(G_{\pi^\pm},\pi^0) \tag{4.87c}$$

$$I^{(4)}(G_{\pi^\pm},\pi^\pm) = B^0\left[\frac{26}{9}-\frac{4}{3}\bar{\ell}_1-\frac{4}{3}\bar{\ell}_2+2\bar{\ell}_3-2\bar{\ell}_4\right]+S^{(4)}(G_{\pi^\pm},\pi^\pm), \tag{4.87d}$$

where $S^{(4)}(G_{\pi^\pm},\pi^0)$, $S^{(4)}(G_{\pi^\pm},\pi^\pm)$ are given in Eq. (D.10). Note that these integrals are related to those of Eq. (4.82) by means of

$$
\begin{aligned}
I^{(j)}(G_{\pi^\pm},\pi^0) &= \frac{1}{2}\,I^{(j)}(G_{\pi^0},\pi^\pm)\\
I^{(j)}(G_{\pi^\pm},\pi^\pm) &= I^{(j)}(G_{\pi^0},\pi^0)+\frac{1}{2}\,I^{(j)}(G_{\pi^0},\pi^\pm),
\end{aligned}
\tag{4.88}
$$

where $j=2,4$. These relations follow from Eq. (4.12) once the pole has been subtracted.

The integrals $I_D^{(2)}(G_{\pi^\pm},\pi^0)$, $I_D^{(2)}(G_{\pi^\pm},\pi^0)$ resp. $I_D^{(2)}(G_{\pi^\pm},\pi^\pm)$, $I_D^{(4)}(G_{\pi^\pm},\pi^\pm)$ can be evaluated from the derivative $\partial_y\mathcal{C}_{\pi^\pm}$. We find

$$I_D^{(2)}(G_{\pi^\pm},\pi^0) = I_D^{(2)}(G_{\pi^\pm},\pi^\pm) = 0 \tag{4.89a}$$

$$I_D^{(4)}(G_{\pi^\pm},\pi^0) = S_D^{(4)}(G_{\pi^\pm},\pi^0) \tag{4.89b}$$

$$I_D^{(4)}(G_{\pi^\pm},\pi^\pm) = S_D^{(4)}(G_{\pi^\pm},\pi^\pm), \tag{4.89c}$$

where $S_D^{(4)}(G_{\pi^\pm},\pi^0)$, $S_D^{(4)}(G_{\pi^\pm},\pi^\pm)$ are given in Eq. (D.11). Note that the above integrals are related to those of masses and of decay constants through

$$\begin{aligned}
I^{(j)}(G_{\pi^\pm},\pi^0) &= I^{(j)}(F_{\pi^\pm},\pi^0) - I^{(j)}(M_{\pi^\pm},\pi^0)\\
I^{(j)}(G_{\pi^\pm},\pi^\pm) &= I^{(j)}(F_{\pi^\pm},\pi^\pm) - I^{(j)}(M_{\pi^\pm},\pi^\pm)\\
I_D^{(j)}(G_{\pi^\pm},\pi^0) &= I_D^{(j)}(F_{\pi^\pm},\pi^0) - I_D^{(j)}(M_{\pi^\pm},\pi^0)\\
I_D^{(j)}(G_{\pi^\pm},\pi^\pm) &= I_D^{(j)}(F_{\pi^\pm},\pi^\pm) - I_D^{(j)}(M_{\pi^\pm},\pi^\pm),
\end{aligned} \tag{4.90}$$

where $j = 2, 4$. These results allow us to check the relations (3.149, 3.150).

The asymptotic formulae for the renormalization terms $\Delta\vartheta^\mu_{\mathscr{G}_{\pi^\pm}}$ read

$$\begin{aligned}
\Delta\vec{\vartheta}_{\mathscr{G}_{\pi^\pm}} &= \vec{R}(\vartheta_{\mathscr{G}_{\pi^\pm}}) + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}})\\
\vec{R}(\vartheta_{\mathscr{G}_{\pi^\pm}}) &= -\frac{1}{2\,(4\pi)^2}\frac{M_\pi}{G_\pi}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\frac{\vec{n}}{|\vec{n}|}\int_{\mathbb{R}} \mathrm{d}y\ \mathrm{e}^{-\lambda_\pi|\vec{n}|\sqrt{1+y^2}}\ y\ \mathcal{K}_{\pi^\pm}(iy,\vartheta_{\pi^+}).
\end{aligned}$$

We insert the chiral representation of $\mathcal{K}_{\pi^\pm}$ obtained from the isospin components (3.131) and expand according to Eq. (4.48b). The asymptotic formulae can be written as

$$\vec{R}(\vartheta_{\mathscr{G}_{\pi^\pm}}) = -\frac{\xi_\pi}{2M_\pi}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\frac{i\vec{n}}{|\vec{n}|}\left[I^{(2)}(\vartheta_{\mathscr{G}_{\pi^\pm}}) + \xi_\pi I^{(4)}(\vartheta_{\mathscr{G}_{\pi^\pm}})\right]\mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}. \tag{4.91}$$

The integrals can be evaluated from the chiral representation of $\mathcal{K}_{\pi^\pm}$. We find

$$I^{(2)}(\vartheta_{\mathscr{G}_{\pi^\pm}}) = 0 \tag{4.92a}$$

$$I^{(4)}(\vartheta_{\mathscr{G}_{\pi^\pm}}) = \pm\left\{-4B^2\left[1-\bar{\ell}_4\right] + S^{(4)}(\vartheta_{\mathscr{G}_{\pi^+}})\right\}, \tag{4.92b}$$

where $S^{(4)}(\vartheta_{\mathscr{G}_{\pi^+}})$ is given in Eq. (D.12). Note that these integrals are related to those of Eqs. (4.66, 4.78) through

$$I^{(j)}(\vartheta_{\mathscr{G}_{\pi^\pm}}) = I^{(j)}(\vartheta_{\mathscr{A}_{\pi^\pm}}) - I^{(j)}(\vartheta_{\Sigma_{\pi^\pm}}), \qquad j = 2, 4. \tag{4.93}$$

These results allow us to check the relations (3.149, 3.150).

4.2.4 Scalar Form Factors at a Vanishing Momentum Transfer

In Section 3.5 we have seen that at a vanishing momentum transfer we can derive asymptotic formulae for the matrix elements of the scalar form factor relying on the Feynman–Hellman Theorem. The formula for the neutral pion reads

$$\begin{aligned}
\delta\Gamma_S^{\pi^0}\big|_{q^2=0} &= R(\Gamma_S^{\pi^0}) + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}})\\
R(\Gamma_S^{\pi^0}) &= -\frac{1}{2\,(4\pi)^2\,\lambda_\pi}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\int_{\mathbb{R}}\frac{\mathrm{d}y}{|\vec{n}|}\,\mathrm{e}^{-\lambda_\pi|\vec{n}|\sqrt{1+y^2}}\\
&\qquad\times\left(1-\lambda_\pi|\vec{n}|\sqrt{1+y^2} + 2M_\pi^2\partial_{M_\pi^2}\right)\mathcal{F}_{\pi^0}(iy,\vartheta_{\pi^+}).
\end{aligned} \tag{4.94}$$

We insert the chiral representation of $\mathcal{F}_{\pi^0}$ obtained from the isospin components (4.4) and expand according to Eq. (4.48a). The asymptotic formula exhibits two contributions,

$$R(\Gamma_S^{\pi^0}) = R(\Gamma_S^{\pi^0}, \pi^0) + R(\Gamma_S^{\pi^0}, \pi^\pm), \tag{4.95}$$

with

$$\begin{aligned} R(\Gamma_S^{\pi^0}, \pi^0) &= -\frac{\xi_\pi}{2\lambda_\pi} \sum_{\substack{\vec{n}\in\mathbb{Z}^3 \\ |\vec{n}|\neq 0}} \frac{1}{|\vec{n}|} \left[I^{(2)}(\Gamma_S^{\pi^0}, \pi^0) + \xi_\pi I^{(4)}(\Gamma_S^{\pi^0}, \pi^0) \right] \\ R(\Gamma_S^{\pi^0}, \pi^\pm) &= -\frac{\xi_\pi}{2\lambda_\pi} \sum_{\substack{\vec{n}\in\mathbb{Z}^3 \\ |\vec{n}|\neq 0}} \frac{1}{|\vec{n}|} \left[I^{(2)}(\Gamma_S^{\pi^0}, \pi^\pm) + \xi_\pi I^{(4)}(\Gamma_S^{\pi^0}, \pi^\pm) \right] \mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}. \end{aligned} \tag{4.96}$$

The integrals $I^{(2)}(\Gamma_S^{\pi^0}, \pi^0)$, $I^{(4)}(\Gamma_S^{\pi^0}, \pi^0)$ resp. $I^{(2)}(\Gamma_S^{\pi^0}, \pi^\pm)$, $I^{(4)}(\Gamma_S^{\pi^0}, \pi^\pm)$ can be evaluated from the chiral representation of $\mathcal{F}_{\pi^0}$. The evaluation involves terms with $\sqrt{1+y^2}\mathcal{F}_{\pi^0}$. For these terms, we make use of

$$\int_{\mathbb{R}} \mathrm{d}y\, y^{2k} \lambda_\pi |\vec{n}| \sqrt{1+y^2}\, \mathrm{e}^{-\lambda_\pi |\vec{n}| \sqrt{1+y^2}} = (2k-1)B^{2k-2} + (2k+1)B^{2k}, \tag{4.97}$$

where B^{2k} are the functions defined in Eq. (4.56). The derivative $\partial_{M_\pi^2}\mathcal{F}_{\pi^0}$ must be evaluated with care. The operator $\partial_{M_\pi^2}$ acts on all quantities depending on the pion mass. For example, it acts on the decay constant F_π and on the constants $\bar{\ell}_j$, see Eq. (4.57). This leads to supplementary terms which must be integrated and added to the results according to their chiral order. Altogether, we find

$$I^{(2)}(\Gamma_S^{\pi^0}, \pi^0) = B^{-2} + 2B^0 \tag{4.98a}$$

$$I^{(2)}(\Gamma_S^{\pi^0}, \pi^\pm) = -2\,[B^{-2} + 2B^0] \tag{4.98b}$$

$$\begin{aligned} I^{(4)}(\Gamma_S^{\pi^0}, \pi^0) = &-B^{-2}\left[\frac{9}{2} - \frac{4}{3}\bar{\ell}_1 - \frac{8}{3}\bar{\ell}_2 + \frac{3}{2}\bar{\ell}_3 - 2\bar{\ell}_4\right] - B^0\left[31 - 8\bar{\ell}_1 - 16\bar{\ell}_2 + 6\bar{\ell}_3 - 4\bar{\ell}_4\right] \\ &+ B^2\left[32 - \frac{16}{3}\bar{\ell}_1 - \frac{32}{3}\bar{\ell}_2\right] + S^{(4)}(\Gamma_S^{\pi^0}, \pi^0) \end{aligned} \tag{4.98c}$$

$$\begin{aligned} I^{(4)}(\Gamma_S^{\pi^0}, \pi^\pm) = &B^{-2}\left[\frac{13}{9} + \frac{8}{3}\bar{\ell}_1 - \bar{\ell}_3 - 4\bar{\ell}_4\right] - B^0\left[2 - \frac{32}{3}\bar{\ell}_1 - \frac{16}{3}\bar{\ell}_2 + 4\bar{\ell}_3 + 8\bar{\ell}_4\right] \\ &+ B^2\left[\frac{176}{9} - \frac{32}{3}\bar{\ell}_2\right] + S^{(4)}(\Gamma_S^{\pi^0}, \pi^\pm), \end{aligned} \tag{4.98d}$$

where $S^{(4)}(\Gamma_S^{\pi^0}, \pi^0)$, $S^{(4)}(\Gamma_S^{\pi^0}, \pi^\pm)$ are explicitly given in Eq. (D.13).

The asymptotic formulae for the matrix elements of the scalar form factor of charged pions read

$$\begin{aligned}
\delta\Gamma_S^{\pi^\pm}\big|_{q^2=0} &= R(\Gamma_S^{\pi^\pm}) + \mathcal{O}(\mathrm{e}^{-\bar\lambda}) \\
R(\Gamma_S^{\pi^\pm}) &= -\frac{1}{2\,(4\pi)^2\,\lambda_\pi} \sum_{\substack{\vec n\in\mathbb{Z}^3\\ |\vec n|\neq 0}} \int_{\mathbb{R}} \frac{\mathrm{d}y}{|\vec n|}\, \mathrm{e}^{-\lambda_\pi |\vec n|\sqrt{1+y^2}} \\
&\quad\times \Bigg[\left(1-\lambda_\pi|\vec n|\sqrt{1+y^2}+2M_\pi^2\partial_{M_\pi^2}\right)\mathcal{F}_{\pi^\pm}(iy,\vartheta_{\pi^+}) \\
&\quad - y\,\frac{D_{\pi^\pm}}{M_\pi}\left(\lambda_\pi|\vec n|\sqrt{1+y^2}+\frac{M_\pi}{M_\pi+D_{\pi^\pm}}-2M_\pi^2\partial_{M_\pi^2}\right)\partial_y\mathcal{F}_{\pi^\pm}(iy,\vartheta_{\pi^+}) \\
&\quad + y\,L\vec n\vec\vartheta_{\pi^\pm}\left(1-\lambda_\pi|\vec n|\sqrt{1+y^2}+2M_\pi^2\partial_{M_\pi^2}\right)\mathcal{G}_{\pi^\pm}(iy,\vartheta_{\pi^+})\Bigg],
\end{aligned} \tag{4.99}$$

where $D_{\pi^\pm}$ is given in Eq. (3.57). We insert the chiral representation of $\mathcal{F}_{\pi^\pm}$, $\mathcal{G}_{\pi^\pm}$ obtained from the isospin components (4.4) and expand according to Eq. (4.48a). The asymptotic formulae exhibit five contributions

$$R(\Gamma_S^{\pi^\pm}) = R(\Gamma_S^{\pi^\pm},\pi^0)+R(\Gamma_S^{\pi^\pm},\pi^\pm)+R_D(\Gamma_S^{\pi^\pm},\pi^0)+R_D(\Gamma_S^{\pi^\pm},\pi^\pm)+2\vec\vartheta_{\pi^\pm}\vec R_{\Gamma_S}(\Theta_{\pi^\pm}), \tag{4.100}$$

where

$$\begin{aligned}
R(\Gamma_S^{\pi^\pm},\pi^0) &= -\frac{\xi_\pi}{2\lambda_\pi}\sum_{\substack{\vec n\in\mathbb{Z}^3\\ |\vec n|\neq 0}}\frac{1}{|\vec n|}\left[I^{(2)}(\Gamma_S^{\pi^\pm},\pi^0)+\xi_\pi I^{(4)}(\Gamma_S^{\pi^\pm},\pi^0)\right] \\
R(\Gamma_S^{\pi^\pm},\pi^\pm) &= -\frac{\xi_\pi}{2\lambda_\pi}\sum_{\substack{\vec n\in\mathbb{Z}^3\\ |\vec n|\neq 0}}\frac{1}{|\vec n|}\left[I^{(2)}(\Gamma_S^{\pi^\pm},\pi^\pm)+\xi_\pi I^{(4)}(\Gamma_S^{\pi^\pm},\pi^\pm)\right]\mathrm{e}^{iL\vec n\vec\vartheta_{\pi^+}} \\
R_D(\Gamma_S^{\pi^\pm},\pi^0) &= -\frac{\xi_\pi}{2\lambda_\pi}\frac{D_{\pi^\pm}}{M_\pi}\sum_{\substack{\vec n\in\mathbb{Z}^3\\ |\vec n|\neq 0}}\frac{1}{|\vec n|}\left[I_D^{(2)}(\Gamma_S^{\pi^\pm},\pi^0)+\xi_\pi I_D^{(4)}(\Gamma_S^{\pi^\pm},\pi^0)\right] \\
R_D(\Gamma_S^{\pi^\pm},\pi^\pm) &= -\frac{\xi_\pi}{2\lambda_\pi}\frac{D_{\pi^\pm}}{M_\pi}\sum_{\substack{\vec n\in\mathbb{Z}^3\\ |\vec n|\neq 0}}\frac{1}{|\vec n|}\left[I_D^{(2)}(\Gamma_S^{\pi^\pm},\pi^\pm)+\xi_\pi I_D^{(4)}(\Gamma_S^{\pi^\pm},\pi^\pm)\right]\mathrm{e}^{iL\vec n\vec\vartheta_{\pi^+}} \\
\vec R_{\Gamma_S}(\Theta_{\pi^\pm}) &= -\frac{\xi_\pi}{4M_\pi}\sum_{\substack{\vec n\in\mathbb{Z}^3\\ |\vec n|\neq 0}}\frac{i\vec n}{|\vec n|}\left[I_{\Gamma_S}^{(2)}(\Theta_{\pi^\pm})+\xi_\pi I_{\Gamma_S}^{(4)}(\Theta_{\pi^\pm})\right]\mathrm{e}^{iL\vec n\vec\vartheta_{\pi^+}}.
\end{aligned} \tag{4.101}$$

The integrals $I^{(2)}(\Gamma_S^{\pi^\pm},\pi^0)$, $I^{(4)}(\Gamma_S^{\pi^\pm},\pi^0)$ resp. $I^{(2)}(\Gamma_S^{\pi^\pm},\pi^\pm)$, $I^{(4)}(\Gamma_S^{\pi^\pm},\pi^\pm)$ can be evaluated from the first group of terms in the square brackets of Eq. (4.99). Using the chiral representation of $\mathcal{F}_{\pi^\pm}$ we find

$$I^{(2)}(\Gamma_S^{\pi^\pm}, \pi^0) = -[B^{-2} + 2B^0] \tag{4.102a}$$

$$I^{(2)}(\Gamma_S^{\pi^\pm}, \pi^\pm) = 0 \tag{4.102b}$$

$$I^{(4)}(\Gamma_S^{\pi^\pm}, \pi^0) = B^{-2}\left[\frac{13}{18} + \frac{4}{3}\bar{\ell}_1 - \frac{1}{2}\bar{\ell}_3 - 2\bar{\ell}_4\right] - B^0\left[1 - \frac{16}{3}\bar{\ell}_1 - \frac{8}{3}\bar{\ell}_2 + 2\bar{\ell}_3 + 4\bar{\ell}_4\right] + B^2\left[\frac{88}{9} - \frac{16}{3}\bar{\ell}_2\right] + S^{(4)}(\Gamma_S^{\pi^\pm}, \pi^0) \tag{4.102c}$$

$$I^{(4)}(\Gamma_S^{\pi^\pm}, \pi^\pm) = -B^{-2}\left[\frac{34}{9} - \frac{8}{3}\bar{\ell}_1 - \frac{8}{3}\bar{\ell}_2 + 2\bar{\ell}_3\right] - B^0\left[32 - \frac{40}{3}\bar{\ell}_1 - \frac{56}{3}\bar{\ell}_2 + 8\bar{\ell}_3\right] + B^2\left[\frac{376}{9} - \frac{16}{3}\bar{\ell}_1 - 16\bar{\ell}_2\right] + S^{(4)}(\Gamma_S^{\pi^\pm}, \pi^\pm), \tag{4.102d}$$

where $S^{(4)}(\Gamma_S^{\pi^\pm}, \pi^0), S^{(4)}(\Gamma_S^{\pi^\pm}, \pi^\pm)$ are given in Eq. (D.14).

The integrals $I_D^{(2)}(\Gamma_S^{\pi^\pm}, \pi^0)$, $I_D^{(4)}(\Gamma_S^{\pi^\pm}, \pi^0)$ resp. $I_D^{(2)}(\Gamma_S^{\pi^\pm}, \pi^\pm)$, $I_D^{(4)}(\Gamma_S^{\pi^\pm}, \pi^\pm)$ can be evaluated from the second group of terms in the square brackets of Eq. (4.99). Here, we must first evaluate the derivative $\partial_y \mathcal{F}_{\pi^\pm}$. We find

$$I_D^{(2)}(\Gamma_S^{\pi^\pm}, \pi^0) = I_D^{(2)}(\Gamma_S^{\pi^\pm}, \pi^\pm) = 0 \tag{4.103a}$$

$$I_D^{(4)}(\Gamma_S^{\pi^\pm}, \pi^0) = -B^0\left[\frac{40}{9} - \frac{16}{3}\bar{\ell}_2\right] + B^2\left[\frac{32}{3} + (1 - C_{\pi^\pm})\left(\frac{40}{9} - \frac{16}{3}\bar{\ell}_2\right)\right] + S_D^{(4)}(\Gamma_S^{\pi^\pm}, \pi^0) \tag{4.103b}$$

$$I_D^{(4)}(\Gamma_S^{\pi^\pm}, \pi^\pm) = -B^0\left[\frac{184}{9} - \frac{16}{3}\bar{\ell}_1 - 16\bar{\ell}_2\right] + B^2\left[\frac{128}{3} + (1 - C_{\pi^\pm})\left(\frac{184}{9} - \frac{16}{3}\bar{\ell}_1 - 16\bar{\ell}_2\right)\right] + S_D^{(4)}(\Gamma_S^{\pi^\pm}, \pi^\pm), \tag{4.103c}$$

where $C_{\pi^\pm} = M_\pi/(M_\pi + D_{\pi^\pm})$ and $S_D^{(4)}(\Gamma_S^{\pi^\pm}, \pi^0)$, $S_D^{(4)}(\Gamma_S^{\pi^\pm}, \pi^\pm)$ are given in Eq. (D.15).

The integrals $I_{\Gamma_S}^{(2)}(\Theta_{\pi^\pm})$, $I_{\Gamma_S}^{(4)}(\Theta_{\pi^\pm})$ can be evaluated from the last group of terms in the square brackets of Eq. (4.99). Using the chiral representation of $\mathcal{G}_{\pi^\pm}$ we find

$$I_{\Gamma_S}^{(2)}(\Theta_{\pi^\pm}) = \pm\left\{4B^0\right\} \tag{4.104a}$$

$$I_{\Gamma_S}^{(4)}(\Theta_{\pi^\pm}) = \pm\left\{-8B^0\left[1 - \bar{\ell}_4\right] + 16B^2 + S_{\Gamma_S}^{(4)}(\Theta_{\pi^+})\right\}, \tag{4.104b}$$

where $S_{\Gamma_S}^{(4)}(\Theta_{\pi^+})$ is given in Eq. (D.16).

4.3 Asymptotic Formulae for Kaons

4.3.1 Masses

The asymptotic formulae for the kaon masses read

$$\begin{aligned}\delta M_{K^\pm} &= R(M_{K^\pm}) + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}})\\ \delta M_{K^0} &= R(M_{K^0}) + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}}),\end{aligned} \tag{4.105}$$

where

$$\begin{aligned}R(M_{K^\pm}) = -\frac{1}{2\,(4\pi)^2\,\lambda_K}\frac{M_\pi}{M_K}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\int_{\mathbb{R}}\frac{\mathrm{d}y}{|\vec{n}|}\,\mathrm{e}^{-\lambda_\pi|\vec{n}|\sqrt{1+y^2}}&\\ \times\left(1+y\frac{D_{K^\pm}}{M_K}\frac{\partial}{\partial y}\right)\mathcal{F}_{K^\pm}(iy,\vartheta_{\pi^+})&\end{aligned} \tag{4.106}$$

$$\begin{aligned}R(M_{K^0}) = -\frac{1}{2\,(4\pi)^2\,\lambda_K}\frac{M_\pi}{M_K}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\int_{\mathbb{R}}\frac{\mathrm{d}y}{|\vec{n}|}\,\mathrm{e}^{-\lambda_\pi|\vec{n}|\sqrt{1+y^2}}&\\ \times\left(1+y\frac{D_{K^0}}{M_K}\frac{\partial}{\partial y}\right)\mathcal{F}_{K^0}(iy,\vartheta_{\pi^+}).&\end{aligned}$$

The parameters $D_{K^\pm}$, D_{K^0} are given in Eq. (3.83). We observe that $R(M_{K^0})$ differs from $R(M_{K^\pm})$ in terms of $D_{K^\pm}$, D_{K^0} and in terms of $\mathcal{F}_{K^\pm}$, $\mathcal{F}_{K^0}$. In Section 4.1.1 we have seen that the chiral representation of $\mathcal{F}_{K^0}$ is equal to that of $\mathcal{F}_{K^-}$, see Eq. (4.25). Hence, we can just consider the asymptotic formulae of charged kaons as in that case, the results of the neutral kaon can be obtained replacing $D_{K^\pm}$ with D_{K^0}.

We insert the chiral representation of $\mathcal{F}_{K^\pm}$ obtained from the isospin components (4.23) in $R(M_{K^\pm})$ and expand according to Eq. (4.48a). The asymptotic formulae of charged kaons exhibit four contributions,

$$R(M_{K^\pm}) = R(M_{K^\pm},\pi^0) + R(M_{K^\pm},\pi^\pm) + R_D(M_{K^\pm},\pi^0) + R_D(M_{K^\pm},\pi^\pm), \tag{4.107}$$

with

$$
\begin{aligned}
R(M_{K^\pm},\pi^0) &= -\frac{\xi_\pi}{2\lambda_\pi}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\frac{1}{|\vec{n}|}\left[I^{(2)}(M_{K^\pm},\pi^0)+\xi_K I^{(4)}(M_{K^\pm},\pi^0)\right]\\
R(M_{K^\pm},\pi^\pm) &= -\frac{\xi_\pi}{2\lambda_\pi}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\frac{1}{|\vec{n}|}\left[I^{(2)}(M_{K^\pm},\pi^\pm)+\xi_K I^{(4)}(M_{K^\pm},\pi^\pm)\right]\mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}\\
R_D(M_{K^\pm},\pi^0) &= -\frac{\xi_\pi}{2\lambda_\pi}\frac{D_{K^\pm}}{M_K}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\frac{1}{|\vec{n}|}\left[I_D^{(2)}(M_{K^\pm},\pi^0)+\xi_K I_D^{(4)}(M_{K^\pm},\pi^0)\right]\\
R_D(M_{K^\pm},\pi^\pm) &= -\frac{\xi_\pi}{2\lambda_\pi}\frac{D_{K^\pm}}{M_K}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\frac{1}{|\vec{n}|}\left[I_D^{(2)}(M_{K^\pm},\pi^\pm)+\xi_K I_D^{(4)}(M_{K^\pm},\pi^\pm)\right]\mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}.
\end{aligned}
\tag{4.108}
$$

The integrals $I^{(2)}(M_{K^\pm},\pi^0)$, $I^{(4)}(M_{K^\pm},\pi^0)$ resp. $I^{(2)}(M_{K^\pm},\pi^\pm)$, $I^{(4)}(M_{K^\pm},\pi^\pm)$ can be evaluated from the chiral representation of $\mathcal{F}_{K^\pm}$. We find

$$I^{(2)}(M_{K^\pm},\pi^0) = I^{(2)}(M_{K^\pm},\pi^\pm) = 0 \tag{4.109a}$$

$$I^{(4)}(M_{K^\pm},\pi^0) = \frac{1}{2}\,I^{(4)}(M_{K^\pm},\pi^\pm) \tag{4.109b}$$

$$
\begin{aligned}
I^{(4)}(M_{K^\pm},\pi^\pm) = 2\,B^0\Bigg[&+8Nx_{\pi K}\,(4L_1^{\mathrm{r}}+L_3^{\mathrm{r}}-4L_4^{\mathrm{r}}-L_5^{\mathrm{r}}+4L_6^{\mathrm{r}}+2L_8^{\mathrm{r}})\\
&+\frac{x_{\pi K}}{9}+\frac{\ell_\pi}{4}\frac{x_{\pi K}^2}{1-x_{\pi K}}\\
&+\frac{\ell_K}{16}\left(\frac{7+x_{\pi K}}{2}-\frac{4}{1-x_{\pi K}}+\frac{1-10x_{\pi K}+x_{\pi K}^2}{6(x_{\eta K}-1)}\right)\\
&+\frac{\ell_\eta}{32}\left(\frac{2}{3}+(1-x_{\pi K})(x_{\eta K}-1)+\frac{53}{9}x_{\pi K}-\frac{x_{\pi K}^2}{3}\right.\\
&\left.-\frac{1-10x_{\pi K}+x_{\pi K}^2}{3(x_{\eta K}-1)}\right)\Bigg]\\
+2\,x_{\pi K}\,B^2\Bigg[&-8N\,(4L_2^{\mathrm{r}}+L_3^{\mathrm{r}})-\frac{\ell_\pi}{2}\frac{5x_{\pi K}}{1-x_{\pi K}}+\frac{\ell_\eta}{2}\frac{x_{\eta K}}{x_{\eta K}-1}\\
&+\frac{\ell_K}{2}\left(\frac{5}{1-x_{\pi K}}-\frac{1}{x_{\eta K}-1}\right)\Bigg]+S^{(4)}(M_{K^\pm},\pi^\pm).
\end{aligned}
\tag{4.109c}
$$

Here, $N=(4\pi)^2$, $\ell_P = 2\log(M_P/\mu)$ and $x_{PQ}=M_P^2/M_Q^2$ for $P,Q=\pi,K,\eta$. The term $S^{(4)}(M_{K^\pm},\pi^\pm)$ is explicitly given in Eq. (D.20). Note that these integrals are related to the integrals $I^{(2)}_{M_K}, I^{(4)}_{M_K}$ of Ref. [32] by virtue of

$$
\begin{aligned}
I^{(j)}(M_{K^\pm}, \pi^0) &= \frac{x_{\pi K}^{-1/2}}{3}\, I^{(j)}_{M_K} \\
I^{(j)}(M_{K^\pm}, \pi^\pm) &= \frac{2}{3} x_{\pi K}^{-1/2}\, I^{(j)}_{M_K},
\end{aligned}
\tag{4.110}
$$

for $j = 2, 4$.

The integrals $I_D^{(2)}(M_{K^\pm}, \pi^0)$, $I_D^{(4)}(M_{K^\pm}, \pi^0)$ resp. $I_D^{(2)}(M_{K^\pm}, \pi^\pm)$, $I_D^{(4)}(M_{K^\pm}, \pi^\pm)$ can be evaluated from the derivative $\partial_y \mathcal{F}_{K^\pm}$. We find

$$
I_D^{(2)}(M_{K^\pm}, \pi^0) = I_D^{(2)}(M_{K^\pm}, \pi^\pm) = 0 \tag{4.111a}
$$

$$
I_D^{(4)}(M_{K^\pm}, \pi^0) = \frac{1}{2}\, I_D^{(4)}(M_{K^\pm}, \pi^\pm) \tag{4.111b}
$$

$$
\begin{aligned}
I_D^{(4)}(M_{K^\pm}, \pi^\pm) = 2\, x_{\pi K} B^2 \Bigg[&- 16N\,(4L_2^{\mathrm{r}} + L_3^{\mathrm{r}}) - \ell_\pi\, \frac{5 x_{\pi K}}{1 - x_{\pi K}} \\
&+ \ell_K \left(\frac{5}{1 - x_{\pi K}} - \frac{1}{x_{\eta K} - 1} \right) \\
&+ \ell_\eta\, \frac{x_{\eta K}}{x_{\eta K} - 1} \Bigg] + S_D^{(4)}(M_{K^\pm}, \pi^\pm),
\end{aligned}
\tag{4.111c}
$$

where $S_D^{(4)}(M_{K^\pm}, \pi^\pm)$ is given in Eq. (D.21).

The asymptotic formulae for the renormalization terms $\Delta\vartheta^\mu_{\Sigma_{K^\pm}}$ read

$$
\begin{aligned}
\Delta\vec{\vartheta}_{\Sigma_{K^\pm}} &= \vec{R}(\vartheta_{\Sigma_{K^\pm}}) + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}}), \\
\vec{R}(\vartheta_{\Sigma_{K^\pm}}) &= -\frac{1}{2\,(4\pi)^2} \frac{M_\pi^2}{M_K} \sum_{\substack{\vec{n}\in\mathbb{Z}^3 \\ |\vec{n}|\neq 0}} \frac{\vec{n}}{|\vec{n}|} \int_{\mathbb{R}} \mathrm{d}y\ \mathrm{e}^{-\lambda_\pi |\vec{n}| \sqrt{1+y^2}}\ y\, \mathcal{G}_{K^\pm}(iy, \vartheta_{\pi^+}).
\end{aligned}
\tag{4.112}
$$

We insert the chiral representation of $\mathcal{G}_{K^\pm}$ obtained from the isospin components (4.23) and expand according to Eq. (4.48b). The asymptotic formulae can be written as

$$
\vec{R}(\vartheta_{\Sigma_{K^\pm}}) = -\frac{\xi_\pi M_K}{2} \sum_{\substack{\vec{n}\in\mathbb{Z}^3 \\ |\vec{n}|\neq 0}} \frac{i\vec{n}}{|\vec{n}|} \left[I^{(2)}(\vartheta_{\Sigma_{K^\pm}}) + \xi_K I^{(4)}(\vartheta_{\Sigma_{K^\pm}}) \right] \mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}. \tag{4.113}
$$

The integrals can be evaluated from the chiral representation of $\mathcal{G}_{K^\pm}$. We find

$$I^{(2)}(\vartheta_{\Sigma_{K^\pm}}) = \pm\left\{-2\,x_{\pi K}^{1/2}\,B^2\right\} \tag{4.114a}$$

$$\begin{aligned} I^{(4)}(\vartheta_{\Sigma_{K^\pm}}) = \pm\Bigg\{ x_{\pi K}^{1/2}\,B^2\Bigg[&-16N x_{\pi K} L_5^{\mathrm{r}} - \frac{\ell_\pi}{2}\frac{5x_{\pi K}^2}{1-x_{\pi K}} \\ &- \frac{\ell_K}{4}\left(7 - \frac{10}{1-x_{\pi K}} + \frac{1+x_{\pi K}}{x_{\eta K}-1}\right) \\ &- \ell_\eta \frac{x_{\eta K}}{4}\left(3 - \frac{1+x_{\pi K}}{x_{\eta K}-1}\right)\Bigg] + S^{(4)}(\vartheta_{\Sigma_{K^+}})\Bigg\}, \end{aligned} \tag{4.114b}$$

where $S^{(4)}(\vartheta_{\Sigma_{K^+}})$ is given in Eq. (D.22). Note that the asymptotic formula for $\Delta\vartheta^\mu_{\Sigma_{K^0}}$ differs from that for $\Delta\vartheta^\mu_{\Sigma_{K^-}}$ only in terms of $\mathcal{G}_{K^0}$, $\mathcal{G}_{K^-}$. As the chiral representation of $\mathcal{G}_{K^0}$ is equal to that of $\mathcal{G}_{K^-}$, the asymptotic formulae are equal in this case, and we can use $\vec{R}(\vartheta_{\Sigma_{K^-}})$ to estimate $\Delta\vartheta^\mu_{\Sigma_{K^0}}$.

4.3.2 Decay Constants of Charged Kaons

The asymptotic formulae for the decay constants of charged kaons read

$$\begin{aligned} \delta F_{K^\pm} &= R(F_{K^\pm}) + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}}) \\ R(F_{K^\pm}) &= \frac{1}{(4\pi)^2\,\lambda_K}\frac{M_\pi}{F_K}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\int_{\mathbb{R}}\frac{\mathrm{d}y}{|\vec{n}|}\,\mathrm{e}^{-\lambda_\pi|\vec{n}|\sqrt{1+y^2}}\left(1 + y\frac{D_{K^\pm}}{M_K}\frac{\partial}{\partial y}\right)\mathcal{N}_{K^\pm}(iy,\vartheta_{\pi^+}), \end{aligned} \tag{4.115}$$

where $D_{K^\pm}$ is given in Eq. (3.83). We insert the chiral representation of $\mathcal{N}_{K^\pm}$ obtained from the isospin components (3.122) and expand according to Eq. (4.48a). The asymptotic formulae exhibit four contributions

$$R(F_{K^\pm}) = R(F_{K^\pm},\pi^0) + R(F_{K^\pm},\pi^\pm) + R_D(F_{K^\pm},\pi^0) + R_D(F_{K^\pm},\pi^\pm), \tag{4.116}$$

where

$$\begin{aligned} R(F_{K^\pm},\pi^0) &= \frac{\xi_\pi}{\lambda_\pi}\frac{F_\pi}{F_K}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\frac{1}{|\vec{n}|}\left[I^{(2)}(F_{K^\pm},\pi^0) + \xi_K I^{(4)}(F_{K^\pm},\pi^0)\right] \\ R(F_{K^\pm},\pi^\pm) &= \frac{\xi_\pi}{\lambda_\pi}\frac{F_\pi}{F_K}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\frac{1}{|\vec{n}|}\left[I^{(2)}(F_{K^\pm},\pi^\pm) + \xi_K I^{(4)}(F_{K^\pm},\pi^\pm)\right]\mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}} \\ R_D(F_{K^\pm},\pi^0) &= \frac{\xi_\pi}{\lambda_\pi}\frac{F_\pi}{F_K}\frac{D_{K^\pm}}{M_K}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\frac{1}{|\vec{n}|}\left[I_D^{(2)}(F_{K^\pm},\pi^0) + \xi_K I_D^{(4)}(F_{K^\pm},\pi^0)\right] \\ R_D(F_{K^\pm},\pi^\pm) &= \frac{\xi_\pi}{\lambda_\pi}\frac{F_\pi}{F_K}\frac{D_{K^\pm}}{M_K}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\frac{1}{|\vec{n}|}\left[I_D^{(2)}(F_{K^\pm},\pi^\pm) + \xi_K I_D^{(4)}(F_{K^\pm},\pi^\pm)\right]\mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}. \end{aligned} \tag{4.117}$$

The integrals $I^{(2)}(F_{K^\pm},\pi^0)$, $I^{(4)}(F_{K^\pm},\pi^0)$ resp. $I^{(2)}(F_{K^\pm},\pi^\pm)$, $I^{(4)}(F_{K^\pm},\pi^\pm)$ can be evaluated from the chiral representation of $\mathcal{N}_{K^\pm}$. We find

$$I^{(2)}(F_{K^\pm},\pi^0) = \frac{1}{2}\, I^{(2)}(F_{K^\pm},\pi^\pm) \tag{4.118a}$$

$$I^{(2)}(F_{K^\pm},\pi^\pm) = -\frac{1}{2}\, B^0 \tag{4.118b}$$

$$I^{(4)}(F_{K^\pm},\pi^0) = \frac{1}{2}\, I^{(4)}(F_{K^\pm},\pi^\pm) \tag{4.118c}$$

$$\begin{aligned} I^{(4)}(F_{K^\pm},\pi^\pm) = 2\Bigg\{ B^0 \Bigg[&+ N\left[4x_{\pi K}(4L_1^{\mathrm{r}} + L_3^{\mathrm{r}} - 2L_4^{\mathrm{r}}) - L_5^{\mathrm{r}}(1+x_{\pi K})\right] \\ &- \ell_\pi\, \frac{x_{\pi K}}{32}\left(7 + \frac{2}{1-x_{\pi K}}\right) + \frac{\ell_K}{16}\left(\frac{1}{1-x_{\pi K}} - \frac{x_{\pi K}}{x_{\eta K}-1}\right) \\ &+ \frac{\ell_\eta}{32}\left(6x_{\pi K} + 3x_{\eta K} + \frac{2x_{\pi K}}{x_{\eta K}-1}\right)\Bigg] \\ + x_{\pi K}\, B^2 \Bigg[&- 8N(4L_2^{\mathrm{r}} + L_3^{\mathrm{r}}) - \frac{\ell_\pi}{2}\,\frac{5x_{\pi K}}{1-x_{\pi K}} \\ &+ \frac{\ell_K}{2}\left(\frac{5}{1-x_{\pi K}} - \frac{1}{x_{\eta K}-1}\right) \\ &+ \frac{\ell_\eta}{2}\,\frac{x_{\eta K}}{x_{\eta K}-1}\Bigg]\Bigg\} + S^{(4)}(F_{K^\pm},\pi^\pm). \end{aligned} \tag{4.118d}$$

The term $S^{(4)}(F_{K^\pm},\pi^\pm)$ is explicitly given in Eq. (D.23). We note that these integrals are related to the integrals $I^{(2)}_{F_K}, I^{(4)}_{F_K}$ of Ref. [32] by virtue of[2]

$$\begin{aligned} I^{(j)}(F_{K^\pm},\pi^0) &= \frac{I^{(j)}_{F_K}}{3} \\ I^{(j)}(F_{K^\pm},\pi^\pm) &= \frac{2}{3}\, I^{(j)}_{F_K}, \end{aligned} \tag{4.119}$$

for $j = 2, 4$.

The integrals $I^{(2)}_D(F_{K^\pm},\pi^0)$, $I^{(4)}_D(F_{K^\pm},\pi^0)$ resp. $I^{(2)}_D(F_{K^\pm},\pi^\pm)$, $I^{(4)}_D(F_{K^\pm},\pi^\pm)$ can be

[2] In Ref. [32] there are two missprints: in Eq. (57) the term $2\ell_\pi(x_{\pi\eta} - \frac{9}{4})$ should read $2(\ell_\eta - \ell_\pi\,\frac{9}{4})$ and in Eq. (79) the factor of $S^{0,4}_{\eta K}$ should read $\frac{3}{32}(1+x_{\pi K})(5-2x_{\pi K}-3x_{\eta K})$ instead of $\frac{3}{32}(5-3x_{\eta K})(1-x^2_{\pi K})$.

evaluated from the derivative $\partial_y \mathcal{N}_{K^\pm}$. We find

$$I_D^{(2)}(F_{K^\pm}, \pi^0) = I_D^{(2)}(F_{K^\pm}, \pi^\pm) = 0 \tag{4.120a}$$

$$I_D^{(4)}(F_{K^\pm}, \pi^0) = \frac{1}{2}\, I_D^{(4)}(F_{K^\pm}, \pi^\pm) \tag{4.120b}$$

$$\begin{aligned} I_D^{(4)}(F_{K^\pm}, \pi^\pm) = 2\, x_{\pi K}\, B^2 \Bigg[&- 16N(4L_2^{\mathrm{r}} + L_3^{\mathrm{r}}) - \ell_\pi \frac{5x_{\pi K}}{1 - x_{\pi K}} \\ &+ \ell_K \left(\frac{5}{1 - x_{\pi K}} - \frac{1}{x_{\eta K} - 1} \right) \\ &+ \ell_\eta \frac{x_{\eta K}}{x_{\eta K} - 1} \Bigg] + S_D^{(4)}(F_{K^\pm}, \pi^\pm), \end{aligned} \tag{4.120c}$$

where $S_D^{(4)}(F_{K^\pm}, \pi^\pm)$ is given in Eq. (D.24).

The asymptotic formulae for the renormalization terms $\Delta\vartheta^\mu_{\mathscr{A}_{K^\pm}}$ read

$$\begin{aligned} \Delta\vec{\vartheta}_{\mathscr{A}_{K^\pm}} &= \vec{R}(\vartheta_{\mathscr{A}_{K^\pm}}) + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}}), \\ \vec{R}(\vartheta_{\mathscr{A}_{K^\pm}}) &= -\frac{1}{2\,(4\pi)^2} \frac{M_\pi^2}{F_K} \sum_{\substack{\vec{n}\in\mathbb{Z}^3 \\ |\vec{n}|\neq 0}} \frac{\vec{n}}{|\vec{n}|} \int_{\mathbb{R}} \mathrm{d}y\ \mathrm{e}^{-\lambda_\pi |\vec{n}| \sqrt{1+y^2}}\ y\ \mathcal{H}_{K^\pm}(iy, \vartheta_{\pi^+}). \end{aligned} \tag{4.121}$$

We insert the chiral representation of $\mathcal{H}_{K^\pm}$ obtained from the isospin components (3.122) and expand according to Eq. (4.48b). The asymptotic formulae can be written as

$$\vec{R}(\vartheta_{\mathscr{A}_{K^\pm}}) = -\frac{\xi_\pi M_K}{2} \frac{F_\pi}{F_K} \sum_{\substack{\vec{n}\in\mathbb{Z}^3 \\ |\vec{n}|\neq 0}} \frac{i\vec{n}}{|\vec{n}|} \left[I^{(2)}(\vartheta_{\mathscr{A}_{K^\pm}}) + \xi_K I^{(4)}(\vartheta_{\mathscr{A}_{K^\pm}}) \right] \mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}. \tag{4.122}$$

The integrals can be evaluated from the chiral representation of $\mathcal{H}_{K^\pm}$. We find

$$I^{(2)}(\vartheta_{\mathscr{A}_{K^\pm}}) = \pm \left\{ -2\, x_{\pi K}^{1/2}\, B^2 \right\} \tag{4.123a}$$

$$\begin{aligned} I^{(4)}(\vartheta_{\mathscr{A}_{K^\pm}}) = \pm \Bigg\{ x_{\pi K}^{1/2}\, B^2 \Bigg[&- 8N x_{\pi K} L_5^{\mathrm{r}} - \frac{\ell_\pi}{4} \frac{5x_{\pi K}^2}{1 - x_{\pi K}} \\ &- \frac{\ell_K}{8} \left(7 - \frac{10}{1 - x_{\pi K}} + \frac{1 + x_{\pi K}}{x_{\eta K} - 1} \right) \\ &- \ell_\eta \frac{x_{\eta K}}{8} \left(3 - \frac{1 + x_{\pi K}}{x_{\eta K} - 1} \right) \Bigg] + S^{(4)}(\vartheta_{\mathscr{A}_{K^+}}) \Bigg\}, \end{aligned} \tag{4.123b}$$

where $S^{(4)}(\vartheta_{\mathscr{A}_{K^+}})$ is given in Eq. (D.25).

4.3.3 Pseudoscalar Coupling Constants of Charged Kaons

The asymptotic formulae for the pseudoscalar coupling constants of charged kaons read

$$\begin{aligned}\delta G_{K^\pm} &= R(G_{K^\pm}) + \mathcal{O}(\mathrm{e}^{-\bar\lambda})\\ R(G_{K^\pm}) &= \frac{1}{(4\pi)^2\lambda_K}\frac{M_\pi M_K}{G_K}\sum_{\substack{\vec n\in\mathbb{Z}^3\\|\vec n|\neq 0}}\int_{\mathbb{R}}\frac{\mathrm{d}y}{|\vec n|}\,\mathrm{e}^{-\lambda_\pi|\vec n|\sqrt{1+y^2}}\\ &\qquad\times\left(1+y\frac{D_{K^\pm}}{M_K}\frac{\partial}{\partial y}\right)\mathcal{C}_{K^\pm}(iy,\vartheta_{\pi^+}).\end{aligned} \tag{4.124}$$

In Section 3.4.2 we have seen that $\mathcal{C}_{K^\pm}$ is related to $\mathcal{F}_{K^\pm}$, $\mathcal{N}_{K^\pm}$ by virtue of Eq. (3.156). We use that relation to determine the chiral representation of $\mathcal{C}_{K^\pm}$ at one loop. If we insert such chiral representation in the asymptotic formulae and expand according to Eq. (4.48a) we obtain

$$R(G_{K^\pm}) = R(G_{K^\pm},\pi^0) + R(G_{K^\pm},\pi^\pm) + R_D(G_{K^\pm},\pi^0) + R_D(G_{K^\pm},\pi^\pm), \tag{4.125}$$

where

$$\begin{aligned} R(G_{K^\pm},\pi^0) &= \frac{\xi_\pi}{\lambda_\pi}\frac{G_\pi}{G_K}\sum_{\substack{\vec n\in\mathbb{Z}^3\\|\vec n|\neq 0}}\frac{1}{|\vec n|}\left[I^{(2)}(G_{K^\pm},\pi^0)+\xi_K I^{(4)}(G_{K^\pm},\pi^0)\right]\\ R(G_{K^\pm},\pi^\pm) &= \frac{\xi_\pi}{\lambda_\pi}\frac{G_\pi}{G_K}\sum_{\substack{\vec n\in\mathbb{Z}^3\\|\vec n|\neq 0}}\frac{1}{|\vec n|}\left[I^{(2)}(G_{K^\pm},\pi^\pm)+\xi_K I^{(4)}(G_{K^\pm},\pi^\pm)\right]\mathrm{e}^{iL\vec n\vec\vartheta_{\pi^+}}\\ R_D(G_{K^\pm},\pi^0) &= \frac{\xi_\pi}{\lambda_\pi}\frac{G_\pi}{G_K}\frac{D_{K^\pm}}{M_K}\sum_{\substack{\vec n\in\mathbb{Z}^3\\|\vec n|\neq 0}}\frac{1}{|\vec n|}\left[I_D^{(2)}(G_{K^\pm},\pi^0)+\xi_K I_D^{(4)}(G_{K^\pm},\pi^0)\right]\\ R_D(G_{K^\pm},\pi^\pm) &= \frac{\xi_\pi}{\lambda_\pi}\frac{G_\pi}{G_K}\frac{D_{K^\pm}}{M_K}\sum_{\substack{\vec n\in\mathbb{Z}^3\\|\vec n|\neq 0}}\frac{1}{|\vec n|}\left[I_D^{(2)}(G_{K^\pm},\pi^\pm)+\xi_K I_D^{(4)}(G_{K^\pm},\pi^\pm)\right]\mathrm{e}^{iL\vec n\vec\vartheta_{\pi^+}}.\end{aligned} \tag{4.126}$$

The integrals can be evaluated from those of Eqs. (4.109, 4.118) by means of

$$\begin{aligned} I^{(j)}(G_{K^\pm},\pi^0) &= \mathring{x}_{\pi K}x_{\pi K}^{-1}\left[I^{(j)}(F_{K^\pm},\pi^0)-\frac{F_K}{F_\pi}I^{(j)}(M_{K^\pm},\pi^0)\right]\\ I^{(j)}(G_{K^\pm},\pi^\pm) &= \mathring{x}_{\pi K}x_{\pi K}^{-1}\left[I^{(j)}(F_{K^\pm},\pi^\pm)-\frac{F_K}{F_\pi}I^{(j)}(M_{K^\pm},\pi^\pm)\right]\\ I_D^{(j)}(G_{K^\pm},\pi^0) &= \mathring{x}_{\pi K}x_{\pi K}^{-1}\left[I_D^{(j)}(F_{K^\pm},\pi^0)-\frac{F_K}{F_\pi}I_D^{(j)}(M_{K^\pm},\pi^0)\right]\\ I_D^{(j)}(G_{K^\pm},\pi^\pm) &= \mathring{x}_{\pi K}x_{\pi K}^{-1}\left[I_D^{(j)}(F_{K^\pm},\pi^\pm)-\frac{F_K}{F_\pi}I_D^{(j)}(M_{K^\pm},\pi^\pm)\right],\end{aligned} \tag{4.127}$$

where $\mathring{x}_{\pi K} = \mathring{M}_\pi^2/\mathring{M}_K^2$ and $j = 2, 4$. These relations follow from Eq. (3.151) and rely on chiral Ward identities. In the evaluation, one must be careful: because of the prefactors (i.e. $\mathring{x}_{\pi K} x_{\pi K}^{-1}$ and F_K/F_π) the integrals with $j = 2$ on the right-hand side generate terms that contribute to the integrals with $j = 4$ on the left-hand side. For the first two types of integrals we find

$$I^{(2)}(G_{K^\pm}, \pi^0) = \frac{1}{2}\, I^{(2)}(G_{K^\pm}, \pi^\pm) \tag{4.128a}$$

$$I^{(2)}(G_{K^\pm}, \pi^\pm) = -\frac{1}{2}\, B^0 \tag{4.128b}$$

$$I^{(4)}(G_{K^\pm}, \pi^0) = \frac{1}{2}\, I^{(4)}(G_{K^\pm}, \pi^\pm) \tag{4.128c}$$

$$\begin{aligned} I^{(4)}(G_{K^\pm}, \pi^\pm) = 2\Bigg\{ B^0 \Bigg[& - N\big[4x_{\pi K}(4L_1^{\mathrm{r}} + L_3^{\mathrm{r}} - 6L_4^{\mathrm{r}} + 8L_6^{\mathrm{r}}) - L_5^{\mathrm{r}}(1 + x_{\pi K})\big] \\ & - 4NL_8^{\mathrm{r}}(1 + 3x_{\pi K}) - \frac{x_{\pi K}}{9} \\ & + \ell_\pi \, \frac{5x_{\pi K}}{32}\left(1 - \frac{2}{1 - x_{\pi K}}\right) \\ & - \frac{\ell_K}{96}\left(21 + 3x_{\pi K} - \frac{30}{1 - x_{\pi K}} + \frac{1 - 4x_{\pi K} + x_{\pi K}^2}{x_{\eta K} - 1}\right) \\ & + \frac{\ell_\eta}{96}\Bigg(+ 1 - 3x_{\pi K} - 6x_{\eta K} + x_{\pi K}^2 + 3x_{\pi K}x_{\eta K} \\ & \qquad + \frac{1 - 4x_{\pi K} + x_{\pi K}^2}{x_{\eta K} - 1}\Bigg)\Bigg]\Bigg\} + S^{(4)}(G_{K^\pm}, \pi^\pm), \end{aligned} \tag{4.128d}$$

where the term $S^{(4)}(G_{K^\pm}, \pi^\pm)$ is given in Eq. (D.26). For the last two types of integrals we find

$$I_D^{(2)}(G_{K^\pm}, \pi^0) = I_D^{(2)}(G_{K^\pm}, \pi^\pm) = 0 \tag{4.129a}$$

$$I_D^{(4)}(G_{K^\pm}, \pi^0) = \frac{1}{2}\, I_D^{(4)}(G_{K^\pm}, \pi^\pm) \tag{4.129b}$$

$$I_D^{(4)}(G_{K^\pm}, \pi^\pm) = S_D^{(4)}(G_{K^\pm}, \pi^\pm), \tag{4.129c}$$

where $S_D^{(4)}(G_{K^\pm}, \pi^\pm)$ is given in Eq. (D.27).

The asymptotic formulae for the renormalization terms $\Delta\vartheta^\mu_{\mathscr{G}_{K^\pm}}$ read

$$\begin{aligned} \Delta\vec{\vartheta}_{\mathscr{G}_{K^\pm}} &= \vec{R}(\vartheta_{\mathscr{G}_{K^\pm}}) + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}}), \\ \vec{R}(\vartheta_{\mathscr{G}_{K^\pm}}) &= -\frac{1}{2\,(4\pi)^2}\frac{M_\pi^2}{G_K M_K}\sum_{\substack{\vec{n}\in\mathbb{Z}^3 \\ |\vec{n}|\neq 0}} \frac{\vec{n}}{|\vec{n}|}\int_{\mathbb{R}} \mathrm{d}y\ \mathrm{e}^{-\lambda_\pi|\vec{n}|\sqrt{1+y^2}}\ y\ \mathcal{K}_{K^\pm}(iy, \vartheta_{\pi^+}). \end{aligned} \tag{4.130}$$

The chiral representation of $\mathcal{K}_{K^\pm}$ is related to that of $\mathcal{G}_{K^\pm}$, $\mathcal{H}_{K^\pm}$ by means of Eq. (3.156). We use that relation to determine the chiral representation of $\mathcal{K}_{K^\pm}$ at one loop. Inserting the representation in the asymptotic formulae and expanding according to Eq. (4.48b) we obtain

$$\vec{R}(\vartheta_{\mathscr{G}_{K\pm}}) = -\frac{\xi_\pi}{2M_K}\frac{G_\pi}{G_K}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\frac{i\vec{n}}{|\vec{n}|}\left[I^{(2)}(\vartheta_{\mathscr{G}_{K\pm}}) + \xi_K I^{(4)}(\vartheta_{\mathscr{G}_{K\pm}})\right]\mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}. \tag{4.131}$$

The integrals can be evaluated from those of Eqs. (4.114, 4.123) by means of

$$I^{(j)}(\vartheta_{\mathscr{G}_{K\pm}}) = \mathring{x}_{\pi K}x_{\pi K}^{-1}\left[I^{(j)}(\vartheta_{\mathscr{A}_{K\pm}}) - \frac{F_K}{F_\pi}I^{(j)}(\vartheta_{\Sigma_{K\pm}})\right], \tag{4.132}$$

where $j = 2, 4$. Here, one must be careful: because of the prefactors (viz. $\mathring{x}_{\pi K}x_{\pi K}^{-1}$ and F_K/F_π) the integrals $I^{(2)}(\vartheta_{\Sigma_{K\pm}})$, $I^{(2)}(\vartheta_{\mathscr{A}_{K\pm}})$ generate terms that contribute to $I^{(4)}(\vartheta_{\mathscr{G}_{K\pm}})$. We find

$$I^{(2)}(\vartheta_{\mathscr{G}_{K\pm}}) = 0 \tag{4.133a}$$

$$\begin{aligned} I^{(4)}(\vartheta_{\mathscr{G}_{K\pm}}) = \pm\Bigg\{ x_{\pi K}^{1/2}\,B^2\Bigg[& + 8NL_5^{\mathrm{r}} + \frac{\ell_\pi}{4}\frac{5x_{\pi K}}{1-x_{\pi K}} \\ & + \frac{\ell_K}{8}\left(3 - \frac{10}{1-x_{\pi K}} + \frac{1+x_{\pi K}}{x_{\eta K}-1}\right) \\ & - \ell_\eta\frac{x_{\eta K}}{8}\left(3 + \frac{1+x_{\pi K}}{x_{\eta K}-1}\right)\Bigg] + S^{(4)}(\vartheta_{\mathscr{G}_{K+}})\Bigg\}, \end{aligned} \tag{4.133b}$$

where $S^{(4)}(\vartheta_{\mathscr{G}_{K+}})$ is given in Eq. (D.28).

4.4 Asymptotic Formula for the Eta Meson

The asymptotic formula for the mass of the eta meson reads

$$\begin{aligned} \delta M_\eta &= R(M_\eta) + \mathcal{O}(\mathrm{e}^{-\bar{\lambda}}) \\ R(M_\eta) &= -\frac{1}{2\,(4\pi)^2\,\lambda_\eta}\frac{M_\pi}{M_\eta}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\int_{\mathbb{R}}\frac{\mathrm{d}y}{|\vec{n}|}\,\mathrm{e}^{-\lambda_\pi|\vec{n}|\sqrt{1+y^2}}\,\mathcal{F}_\eta(iy,\vartheta_{\pi^+}). \end{aligned} \tag{4.134}$$

We insert the chiral representation of $\mathcal{F}_\eta$ obtained from the isospin components (4.39) and expand according to Eq. (4.48a). The asymptotic formula exhibits two contributions

$$R(M_\eta) = R(M_\eta,\pi^0) + R(M_\eta,\pi^\pm) \tag{4.135}$$

with

$$
\begin{aligned}
R(M_\eta,\pi^0) &= -\frac{\xi_\pi}{2\lambda_\pi}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\frac{1}{|\vec{n}|}\left[I^{(2)}(M_\eta,\pi^0)+\xi_\eta I^{(4)}(M_\eta,\pi^0)\right]\\
R(M_\eta,\pi^\pm) &= -\frac{\xi_\pi}{2\lambda_\pi}\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}}\frac{1}{|\vec{n}|}\left[I^{(2)}(M_\eta,\pi^\pm)+\xi_\eta I^{(4)}(M_\eta,\pi^\pm)\right]\mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}}.
\end{aligned}
\tag{4.136}
$$

The integrals $I^{(2)}(M_\eta,\pi^0)$, $I^{(4)}(M_\eta,\pi^0)$ resp. $I^{(2)}(M_\eta,\pi^\pm)$, $I^{(4)}(M_\eta,\pi^\pm)$ can be evaluated from the chiral representation of $\mathcal{F}_\eta$. We find

$$I^{(2)}(M_\eta,\pi^0) = \frac{1}{2}\,I^{(2)}(M_\eta,\pi^\pm) \tag{4.137a}$$

$$I^{(2)}(M_\eta,\pi^\pm) = \frac{2}{3}x_{\pi\eta}\,B^0 \tag{4.137b}$$

$$I^{(4)}(M_\eta,\pi^0) = \frac{1}{2}\,I^{(4)}(M_\eta,\pi^\pm) \tag{4.137c}$$

$$
\begin{aligned}
I^{(4)}(M_\eta,\pi^\pm) = \frac{2}{3}x_{\pi\eta}\Bigg\{ B^0\Bigg[&+16N\big(6\,(L_1^{\mathrm{r}}-L_4^{\mathrm{r}}+L_6^{\mathrm{r}}-L_7^{\mathrm{r}})+L_3^{\mathrm{r}}-L_5^{\mathrm{r}}\big)\\
&+16N x_{\pi\eta}\,(6L_7^{\mathrm{r}}+3L_8^{\mathrm{r}})\\
&-\ell_\pi\,\frac{x_{\pi\eta}}{3}\left(\frac{13}{2}-\frac{2}{1-x_{\pi\eta}}\right)+\ell_K\,(2x_{K\eta}-x_{\pi\eta})\\
&+\frac{\ell_\eta}{3}\left(\frac{x_{\pi\eta}}{2}-\frac{2}{1-x_{\pi\eta}}\right)-\frac{2+x_{\pi\eta}}{3}\Bigg]\\
+B^2\Big[-32N\,(3L_2^{\mathrm{r}}+L_3^{\mathrm{r}})&+9\,(1+\ell_K)\Big]\Bigg\}+S^{(4)}(M_\eta,\pi^\pm),
\end{aligned}
\tag{4.137d}
$$

where $S^{(4)}(M_\eta,\pi^\pm)$ is explicitly given in Eq. (D.29). Note that these integrals are related to the integrals $I^{(2)}_{M_\eta}, I^{(4)}_{M_\eta}$ of Ref. [32] by virtue of

$$
\begin{aligned}
I^{(j)}(M_\eta,\pi^0) &= \frac{x_{\pi\eta}^{-1/2}}{3}\,I^{(j)}_{M_\eta}\\
I^{(j)}(M_\eta,\pi^\pm) &= \frac{2}{3}x_{\pi\eta}^{-1/2}\,I^{(j)}_{M_\eta},
\end{aligned}
\tag{4.138}
$$

for $j=2,4$.

Chapter 5

Numerical Results

We estimate finite volume corrections numerically with the formulae presented in Chapters 2 and 4. We first adopt the numerical set-up of Ref. [25, 32] and perform a generic analysis. The numerical results are presented at NLO in Section 5.2 and beyond that order in Section 5.3. In Section 5.4, we then take lattice data from two collaborations [49–51] and illustrate how the formulae can be possibly applied to real simulations. The results show that finite volume corrections can be comparable (or even larger) than the statistical precision of lattice simulations. Hence, they should be taken into account before results of lattice extrapolations can be compared with experimental measurements.

5.1 Numerical Set-up of Generic Analysis

We adopt the numerical set-up of Ref. [25,32] and express the quantities in infinite volume appearing in the formulae (i.e. F_π, F_K, M_K, M_η) as functions of M_π. For F_π we use the expression at NNLO obtained with 2-light-flavor ChPT while for F_K, M_K, M_η we use expressions at NLO of 3-light-flavor ChPT. In any cases, the values of the relevant LEC are summarized in Tab. 5.1. If avalaible, these values are taken from results of lattice simulations with $N_\mathrm{f} = 2+1$ dynamical flavors. For LEC of 2-light-flavor ChPT we take the averages of the FLAG working group [86] which are obtained from Ref. [87, 89, 138, 139]. For LEC of 3-light-flavor ChPT we take the results of Ref. [137] as recommended by FLAG [86]. The remaining values come from phenomenology [135, 136] or have been determined evaluating the expressions of F_π, F_K, M_K, M_η at the physical point (see later). For each LEC, we quote the review articles they are taken from.

Table 5.1: Values of the relevant LEC used in the numerical analysis. The values of LEC refer to the renormalization scale $\mu = 0.770$ GeV. Note that the central value of L_7^{r} has been determined evaluating the expression of the mass of the eta meson at the physical point (see text). The uncertainity on L_7^{r} has been taken as in Tab. 5 (column "All") of Ref. [135].

(a) 2-light-flavor LEC.

j	$\bar{\ell}_j^{\mathrm{phys}}$	Ref.
1	-0.36 ± 0.59	[136]
2	4.31 ± 0.11	[136]
3	3.05 ± 0.99	[86]
4	4.02 ± 0.28	[86]

(b) 3-light-flavor LEC.

j	$L_j^{\mathrm{r}}(\mu) \cdot 10^3$	Ref.
1	0.88 ± 0.09	[135]
2	0.61 ± 0.20	[135]
3	-3.04 ± 0.43	[135]
4	0.04 ± 0.14	[137]
5	0.84 ± 0.38	[137]
6	0.07 ± 0.10	[137]
7	-0.16 ± 0.15	
8	0.36 ± 0.09	[137]

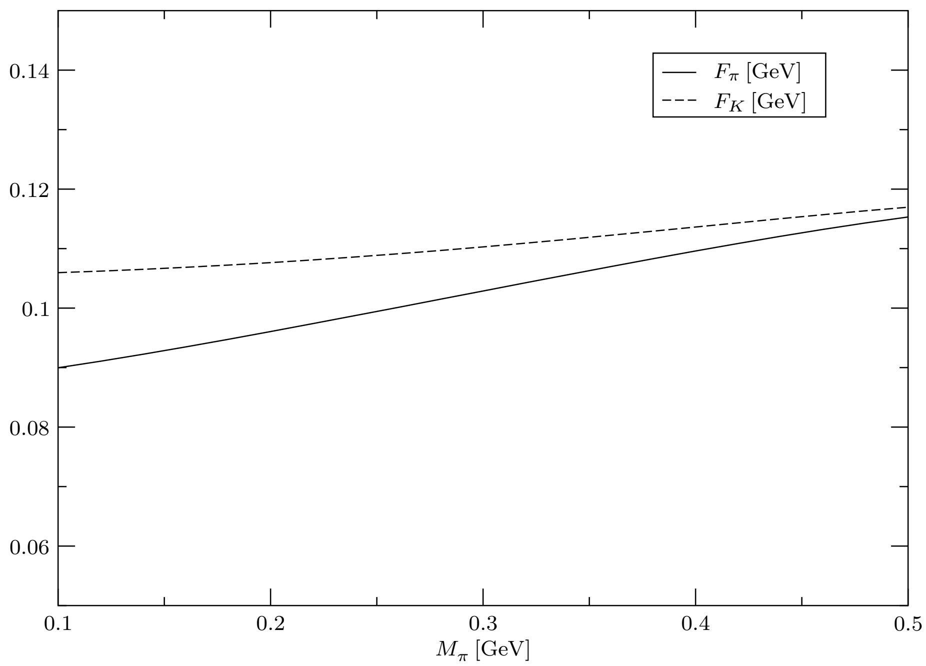


Figure 5.1: Pion mass dependence of F_π, F_K in infinite volume.

5.1.1 Pion Mass Dependence in Infinite Volume

In infinite volume, the expression of the pion decay constant at NNLO reads

$$F_\pi = F\left\{1+\xi\bar{\ell}_4+\xi^2\left[\frac{5}{4}\ell_\pi^2+\ell_\pi\left(\frac{7}{6}\bar{\ell}_1+\frac{4}{3}\bar{\ell}_2+\frac{\bar{\ell}_3}{2}-\frac{\bar{\ell}_4}{2}+2\right)\right.\right.$$
$$\left.\left.+\frac{\bar{\ell}_3}{2}\bar{\ell}_4-\frac{\bar{\ell}_1}{12}-\frac{\bar{\ell}_2}{3}-\frac{13}{192}+r_F(\mu)\right]\right\}. \quad (5.1)$$

This expression is obtained with 2-light-flavor ChPT, see Ref. [115]. Here, $\xi = M_\pi^2/(4\pi F)^2$ and $\ell_\pi = 2\log(M_\pi/\mu)$. The constants $\bar{\ell}_j$ are given in Eq. (4.57) and the values of $\bar{\ell}_j^{\text{phys}}$ are summarized in Tab. 5.1. The parameter $r_F(\mu)$ is a combination of LEC at NNLO. In Ref. [25] it was estimated as $r_F(\mu) = 0 \pm 3$.

We can determine F numerically, evaluating Eq. (5.1) at the physical point. Taking $M_\pi = M_{\pi^\pm}^{\text{phys}}$ and inverting the expression, we find

$$F = (86.6 \pm 0.4)\ \text{MeV}. \quad (5.2)$$

This value agrees with the result of Ref. [25] and provides the ratio $F_\pi/F = (1.065\pm 0.006)$ which in turn agrees with the FLAG average obtained from simulations with $N_{\text{f}} = 2+1$ dynamical flavors, see Ref. [86, 89, 137, 139].

In Fig. 5.1 we represent the pion mass dependence of decay constants. We observe that the dependence of F_π is rather mild. As in Ref. [25], we conclude that this dependence is too mild to violate the condition of Eq. (2.3). Thus, we can rely on ChPT and apply the formulae of Chapters 2 and 4 to estimate finite volume corrections.

In infinite volume, the expressions at NLO of M_K^2, M_η^2, F_K obtained with 3-light-flavor ChPT read

$$M_K^2 = \mathring{M}_K^2 + \frac{1}{F_\pi^2}\left\{M_\pi^4\left[-2k_1+\frac{1}{4N}\left(-\ell_\pi+\mathring{\ell}_\eta/3\right)\right]\right.$$
$$\left.+\, m_sB_0\left(M_\pi^2+m_sB_0\right)\left[8(k_1+2k_2)+\frac{4}{9N}\mathring{\ell}_\eta\right]\right\} \quad (5.3a)$$

$$M_\eta^2 = \mathring{M}_\eta^2 + \frac{1}{F_\pi^2}\left\{M_\pi^4\left[\frac{161}{9}(-k_1+2k_3)+\frac{1}{3N}(-2\ell_\pi+\mathring{\ell}_K)\right]\right.$$
$$\left.+\, M_\pi^2 m_sB_0\left[\frac{64}{9}(k_1+3k_2-2k_3)\frac{4}{3N}\left(\mathring{\ell}_K-\frac{2}{9}\mathring{\ell}_\eta\right)\right]\right\} \quad (5.3b)$$

$$F_K = F_\pi + \frac{1}{F_\pi^2}\left[4(M_K^2-M_\pi^2)L_5^{\text{r}}+\frac{1}{N}\left(\frac{5}{8}M_\pi^2\ell_\pi-\frac{1}{4}M_K^2\ell_\eta-\frac{3}{8}M_\eta^2\ell_\eta\right)\right], \quad (5.3c)$$

see Ref. [32]. In these expressions, $\mathring{\ell}_P = 2\log(\mathring{M}_P/\mu)$ resp. $\ell_P = 2\log(M_P/\mu)$ for $P = \pi, K, \eta$ and

$$k_1 = 2L_8^{\text{r}} - L_5^{\text{r}} \qquad k_2 = 2L_6^{\text{r}} - L_4^{\text{r}} \qquad k_3 = 3L_7^{\text{r}} + L_8^{\text{r}}, \quad (5.4)$$

are linear combinations of 3-light-flavor LEC. The decay constant F_π is expressed as in Eq. (5.1). Here, the circled masses are not just at leading order but they have an hybrid nature,

$$\overset{\circ}{M}{}_K^2 = \frac{1}{2}(M_\pi^2 + 2B_0 m_s) \qquad \overset{\circ}{M}{}_\eta^2 = \frac{1}{3}(M_\pi^2 + 4B_0 m_s). \tag{5.5}$$

The part containing M_π^2 is at NLO while the part containing $B_0 m_s$ is at leading order. This is unavoidable if we want to study the dependence on the pion mass of M_K, M_η, F_K in ChPT. In practice, we use the first two expressions (5.3a, 5.3b) to determine $B_0 m_s$, L_7^{r} and the third one (5.3c) to check the numerical results.

Taking the values of LEC from Tab. 5.1 we evaluate the first expression (5.3a) at $M_\pi = M_{\pi^\pm}^{\mathrm{phys}}$. Requiring $M_K = M_{K^\pm}^{\mathrm{phys}}$ we find $B_0 m_s = 0.241\ \mathrm{GeV}^2$. The uncertainity on this value is of order $10^{-5}\ \mathrm{GeV}^2$ and may be neglected. In a similar way, we evaluate the second expression (5.3b) at $M_\pi = M_{\pi^\pm}^{\mathrm{phys}}$ and require $M_\eta = M_\eta^{\mathrm{phys}}$. We find $L_7^{\mathrm{r}} = -0.16 \cdot 10^{-3}$. This value agrees with the result presented in Tab. 5 (column "All") of Ref. [135]. As the uncertainity estimated through Eq. (5.3b) is $\mathcal{O}(10^{-7})$ we decide to take the uncertainity given in Ref. [135]. This yields $L_7^{\mathrm{r}} = (-0.16 \pm 0.15) \cdot 10^{-3}$. To check our numerical results on $B_0 m_s$, L_7^{r} we insert the expressions of $\overset{\circ}{M}{}_K^2$, $\overset{\circ}{M}{}_\eta^2$ in Eq. (5.3c) and evaluate F_K at $M_\pi = M_{\pi^\pm}^{\mathrm{phys}}$. We find

$$F_K = (0.106 \pm 0.004)\ \mathrm{GeV}. \tag{5.6}$$

Such value agrees with the result of PDG [2] and with the FLAG average obtained from simulations with $N_{\mathrm{f}} = 2 + 1$ dynamical flavors, see Ref. [86, 138, 140, 141].

We stress that here, F_π is expressed with 2-light-flavor ChPT even in the 3-light-flavor expressions of M_K^2, M_η^2, F_K. This choice was already made in Ref. [32] and for $m_s = m_s^{\mathrm{phys}}$ it exacty reproduces what one would get in the 3-light-flavor framework[1]. As lattice simulations are usually performed at $m_s \approx m_s^{\mathrm{phys}}$ we expect that such choice remains a valid approximation also in our numerical analysis.

In Fig. 5.2 we represent the pion mass dependence of M_K, M_η. We observe that the dependence on M_π is mild. The same holds for F_K as one sees from Fig. 5.1. Note that for $M_\pi \approx 0.500$ GeV we have $M_K \approx 0.610$ GeV and $M_\eta \approx 0.640$ GeV. In that case, the values of M_π, M_K, M_η are all similar. If we consider $\xi_P = M_P^2/(4\pi F_\pi)^2$ for $P = \pi, K, \eta$ we expect that these parameters stay small for all pion masses in $[0.1\ \mathrm{GeV}, 0.5\ \mathrm{GeV}]$. This is confirmed by Fig. 5.3 where the pion mass dependence of ξ_P is represented graphically. In the numerical analysis we will use the expansion parameters exactly as in Fig. 5.3. In particular, we will consider ξ_P as exact and ignore their uncertainities. This choice is justified by the fact that in lattice simulations such parameters can be determined iteratively from $M_P^2(L)/[4\pi F_{\pi^\pm}(L)]^2$ where the values of $M_P(L)$, $F_{\pi^\pm}(L)$ may be refined applying asymptotic formulae.

[1] Indeed, the low-energy constants $\bar{\ell}_j$ encode information about the virtual s-quark.

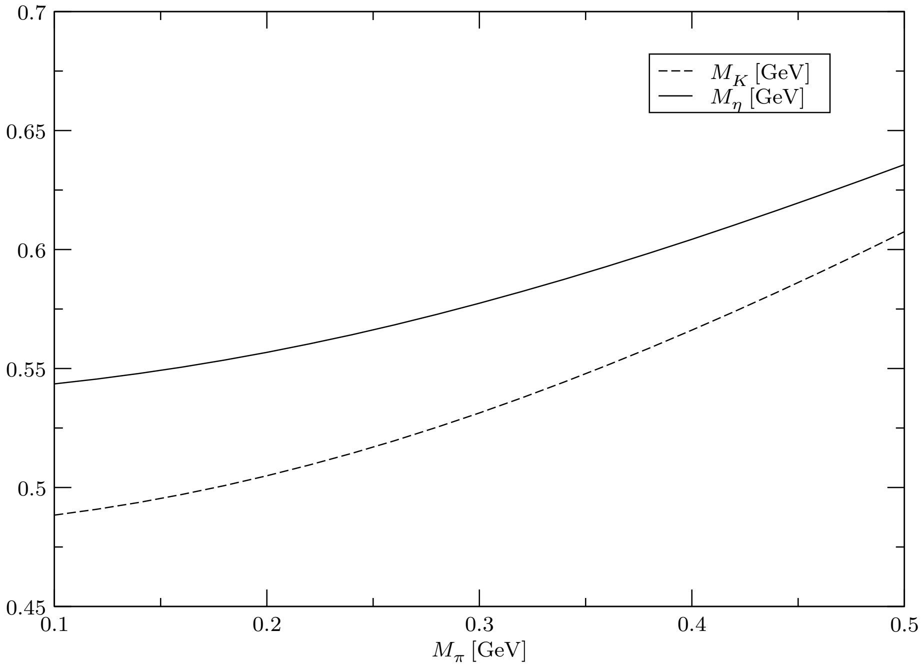


Figure 5.2: Pion mass dependence of M_K, M_η in infinite volume.

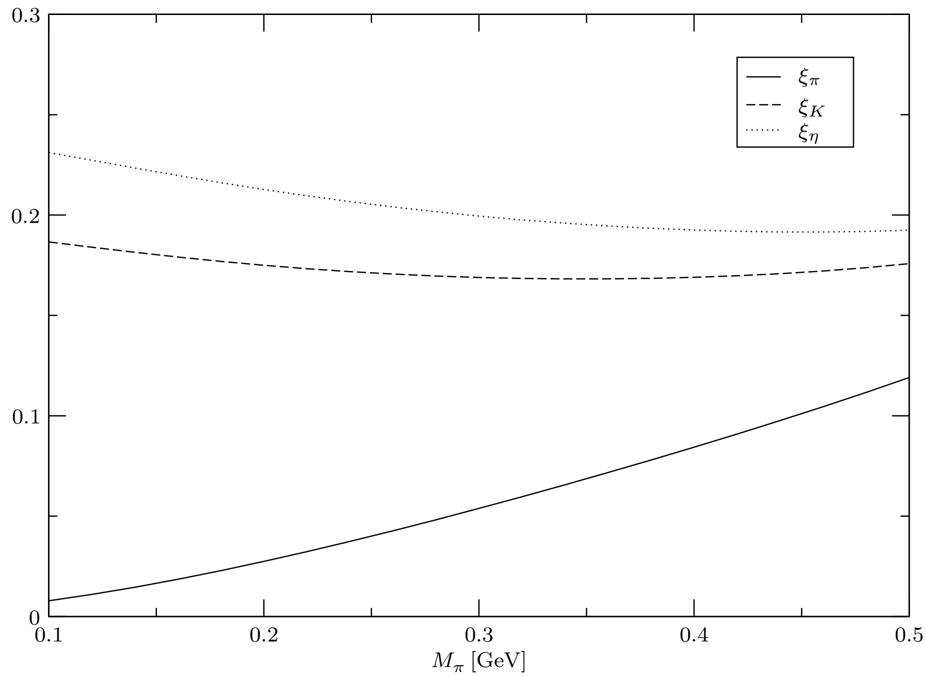


Figure 5.3: Pion mass dependence of ξ_P in infinite volume.

5.1.2 Twisting Angles, Multiplicity and Presentation of Results

In simulations of Lattice QCD, twisted boundary conditions are usually imposed in just one spatial direction. In that case, the twisting angles are aligned to a specific axis. Furthermore, it is usual to impose TBC on just one flavor, e.g. on the u-quark. Then, the twisting angles result

$$\vec{\vartheta}_u = \frac{1}{L}\begin{pmatrix}\theta\\0\\0\end{pmatrix} \qquad \text{resp.} \qquad \vec{\vartheta}_d = \vec{\vartheta}_s = \vec{0}. \tag{5.7}$$

We use this configuration of twisting angles to perform the numerical analysis. In principle, the angle θ can be arbitrarly chosen. Since we rely on ChPT, we require $\theta/L \ll 4\pi F_\pi$. If we consider $L \gg 1$ fm –as requested by Eq. (2.3)– the condition $\theta/L \ll 4\pi F_\pi$ is certainly satisfied for $\theta \in [0, 2\pi]$. Note that in the effective theory, the configuration (5.7) implies that the twisting angles of charged pions and charged kaons are equal whereas that of the neutral kaon is zero: $\vec{\vartheta}_{\pi^+} = \vec{\vartheta}_{K^+} = \vec{\vartheta}_u$ resp. $\vec{\vartheta}_{K^0} = \vec{0}$. Obviously, this simplifies a lot of calculations and allows us to study the dependence on twisting angles just by varying θ.

The configuration (5.7) is convenient for an other aspect. As twisting angles are aligned to one specific axis, we may use the formula,

$$\sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}} f(\,|\vec{n}|\,)\,\mathrm{e}^{iL\vec{n}\vec{\vartheta}_{\pi^+}} = \sum_{n=1}^{\infty} f(\sqrt{n}\,) \sum_{n_1=-\lfloor\sqrt{n}\rfloor}^{\lfloor\sqrt{n}\rfloor} m(n,n_1)\,\mathrm{e}^{in_1\theta}, \tag{5.8}$$

to rewrite the three sums over the integer winding numbers as a nested sum over $n \in \mathbb{N}$. In general, this speeds up the numerical evaluation by a factor 15. The notation $\lfloor\,.\,\rfloor$ indicates the floor function, namely $\lfloor x\rfloor$ is the largest integer number not greater than $x \in \mathbb{R}$. The factor $m(n, n_1)$ is called multiplicity. It corresponds to the number of possibilities to construct a vector $\vec{n} \in \mathbb{Z}^3$ with $n = |\vec{n}|^2$, having previously fixed the value of the first component to $n_1 \in \mathbb{Z}$. In Tab. 5.2 we list the values of the multiplicity for $n \leq 30$. Note that the prefactor 6 in the asymptotic formulae (3.1, 3.2) corresponds to the sum of the multiplicity of a vector with $n = 1$.

In Sections 5.2 and 5.3 we present numerical results by means of graphs. We plot the dependences on the pion mass M_π and on the angle θ of the corrections. The pion mass dependence is plotted for different values of the side length L and of the angle θ. Lines of different colors refer to different values of L: black lines ($L = 2$ fm), green lines ($L = 3$ fm), red lines ($L = 4$ fm). Lines of different hatchings refer to different values of θ: solid lines ($\theta = 0$), dashed lines ($\theta = \pi/8$), dot-dashed lines ($\theta = \pi/4$), dotted lines ($\theta = \pi/3$). The dark (resp. light) yellow areas refer to the region $M_\pi L < 2$ for $\theta = 0$ (resp. $\theta = \pi/3$).

The angle dependence is plotted for different values of the pion mass M_π and at a fixed side length. Lines of different hatchings refer to different values of M_π: solid lines ($M_\pi = 0.140$ GeV), dashed lines ($M_\pi = 0.197$ GeV), dot-dashed lines ($M_\pi = 0.240$ GeV), dotted lines ($M_\pi = 0.340$ GeV). Note that if we take $L = 2$ fm, the region $M_\pi L < 2$ begins

Table 5.2: Multiplicity of vectors $\vec{n} \in \mathbb{Z}^3$ with $n := |\vec{n}|^2 \leq 30$.

$m(n, n_1)$ n_1 / n	0	± 1	± 2	± 3	± 4	± 5
1	4	1	0	0	0	0
2	4	4	0	0	0	0
3	0	4	0	0	0	0
4	4	0	1	0	0	0
5	8	4	4	0	0	0
6	0	8	4	0	0	0
7	0	0	0	0	0	0
8	4	0	4	0	0	0
9	4	4	8	1	0	0
10	8	4	0	4	0	0
11	0	8	0	4	0	0
12	0	0	4	0	0	0
13	8	0	4	4	0	0
14	0	8	8	8	0	0
15	0	0	0	0	0	0
16	4	0	0	0	1	0
17	8	4	8	4	4	0
18	4	8	0	4	4	0
19	0	4	0	8	0	0
20	8	0	4	0	4	0
21	0	8	8	0	8	0
22	0	0	4	8	0	0
23	0	0	0	0	0	0
24	0	0	8	0	4	0
25	12	0	0	4	4	1
26	8	12	0	8	8	4
27	0	8	0	4	0	4
28	0	0	0	0	0	0
29	8	0	12	8	8	4
30	0	8	8	0	0	8

for masses smaller than $M_\pi = 0.197$ GeV. We remind that in that region, numerical results should be taken with a grain of salt as the p-regime is no more guaranteed.

5.2 Finite Volume Corrections at NLO

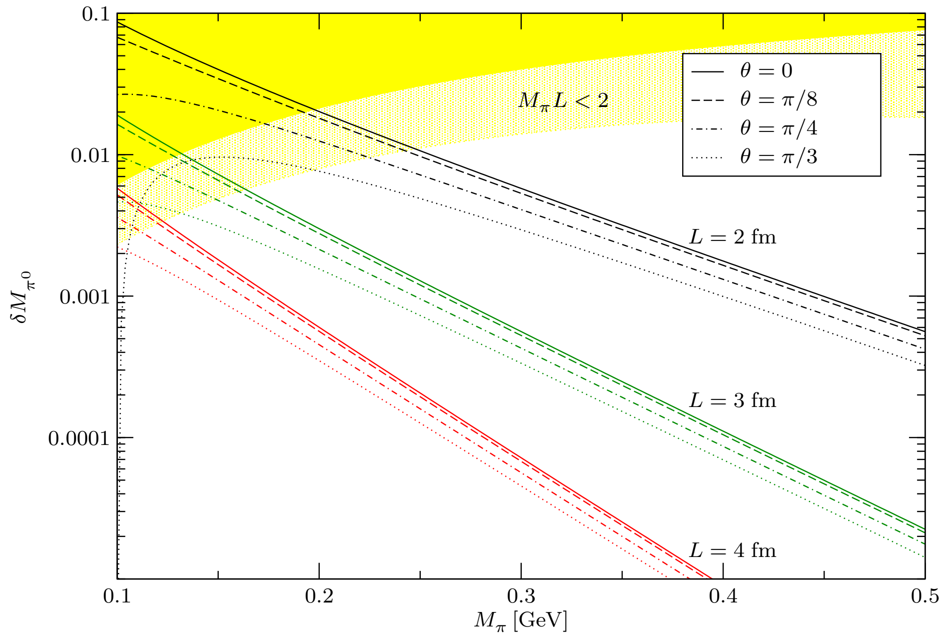
5.2.1 Masses and Renormalization Terms

Masses

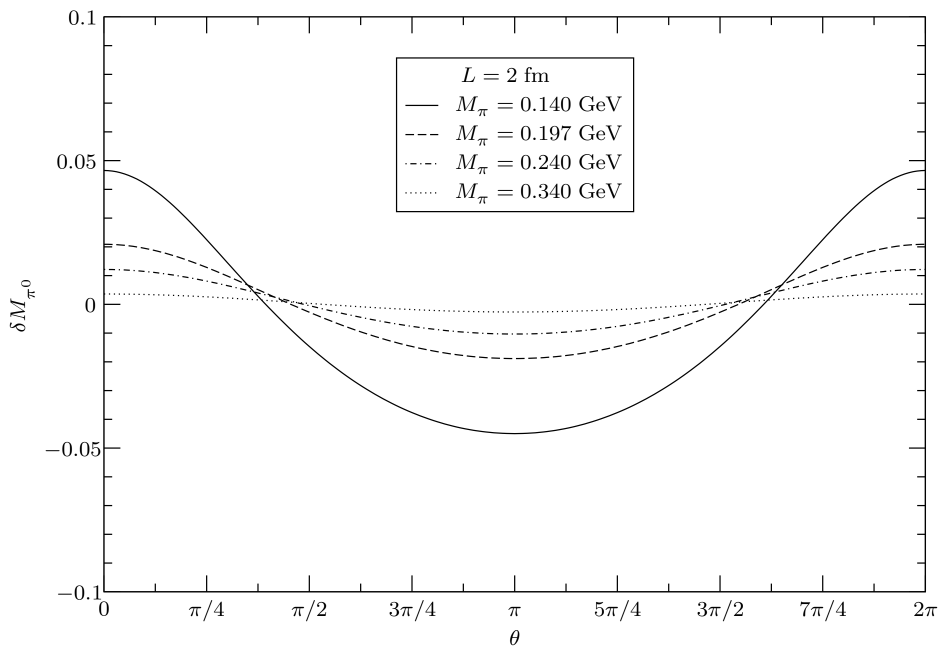
We begin with the mass corrections at NLO. At this order, only δM_{π^0}, δM_η exhibit a dependence on twisting angles. The corrections $\delta M_{\pi^\pm}$, $\delta M_{K^\pm}$, δM_{K^0} do not depend on the twist. Moreover, $\delta M_{K^0} = \delta M_{K^\pm}$ and $\delta M_{\pi^\pm}$ is given by δM_{π^0} evaluated at $\theta = 0$, see Eq. (2.43). Hence, we concentrate on δM_{π^0}, $\delta M_{K^\pm}$, δM_η and disregard $\delta M_{\pi^\pm}$, δM_{K^0}.

In Fig. 5.4 and 5.5 we represent the dependences on M_π and on θ. The pion mass dependence of δM_{π^0} is represented in a logarithmic graph (see Fig. 5.4a) whereas the pion mass dependences of $\delta M_{K^\pm}$, δM_η in a linear graph (see Fig. 5.5a). The logarithmic graph illustrates the exponential decay in M_π of δM_{π^0}. The corrections decay as $\mathcal{O}(\mathrm{e}^{-M_\pi L})$ and are represented by almost straight lines. In general, the corrections are positive and for $\theta \in \{0, \pi/8, \pi/4, \pi/3\}$ their absolute values decrease with the angle. If we consider $L = 2$ fm we read that δM_{π^0} is about 2.1% for $\theta = 0$ (resp. 0.8% for $\theta = \pi/3$) at $M_\pi \approx 0.2$ GeV and decreases to less than 0.1% at $M_\pi \approx 0.5$ GeV. Considering the same side length, δM_η is one order of magnitude less and $\delta M_{K^\pm}$ is even smaller, see Fig. 5.5a. Moreover, δM_η is negative for $M_\pi \in [0.1 \text{ GeV}, 0.5 \text{ GeV}]$ and $\delta M_{K^\pm}$ is nearly constant in the same interval. All these features can be explained if we look the expressions of the mass corrections at NLO, see Eq. (2.43). At this order, δM_η has various contributions of which the dominant one is that of virtual pions. In the expression (2.43d) the contribution of virtual pions is suppressed by a factor $-M_\pi^2/M_\eta^2$. This factor suppresses the mass corrections of the eta meson with respect to δM_{π^0} and makes δM_η negative. At NLO $\delta M_{K^\pm}$ has just one contribution due to the virtual eta meson. This contribution decays as $\mathcal{O}(\mathrm{e}^{-M_\eta L})$ and is nearly constant because of the slow variation of the eta mass in infinite volume, see Fig. 5.2. As consequences, $\delta M_{K^\pm}$ is much smaller than δM_{π^0} and nearly constant for $M_\pi \in [0.1 \text{ GeV}, 0.5 \text{ GeV}]$.

In Fig. 5.4b we represent the angle dependence of δM_{π^0}. We observe that δM_{π^0} depends on θ as a cosinus function. The corrections oscillate with a period of 2π and have maxima (resp. minima) at even (resp. odd) integer multiples of π. If we consider $M_\pi = 0.197$ GeV, the difference among maxima and minima is 4.0% at $L = 2$ fm. This is a sizable effect which should be taken into account when physical observables are extrapolated from lattice data. Note that δM_{π^0} turns negative for $\theta \in [3\pi/8, 13\pi/8]$ unlike the case of PBC (i.e. $\theta = 0$) where it is always positive. In the same graph, $\delta M_{\pi^\pm}$ would be constant and would value as δM_{π^0} at $\theta = 0$. In Fig. 5.5b we represent the angle dependences of $\delta M_{K^\pm}$, δM_η. We observe that $\delta M_{K^\pm}$ is constant and δM_η depends on θ as a negative cosinus function. Considering $M_\pi = 0.197$ GeV, the difference among maxima and minima in δM_η is 0.1% at $L = 2$ fm.

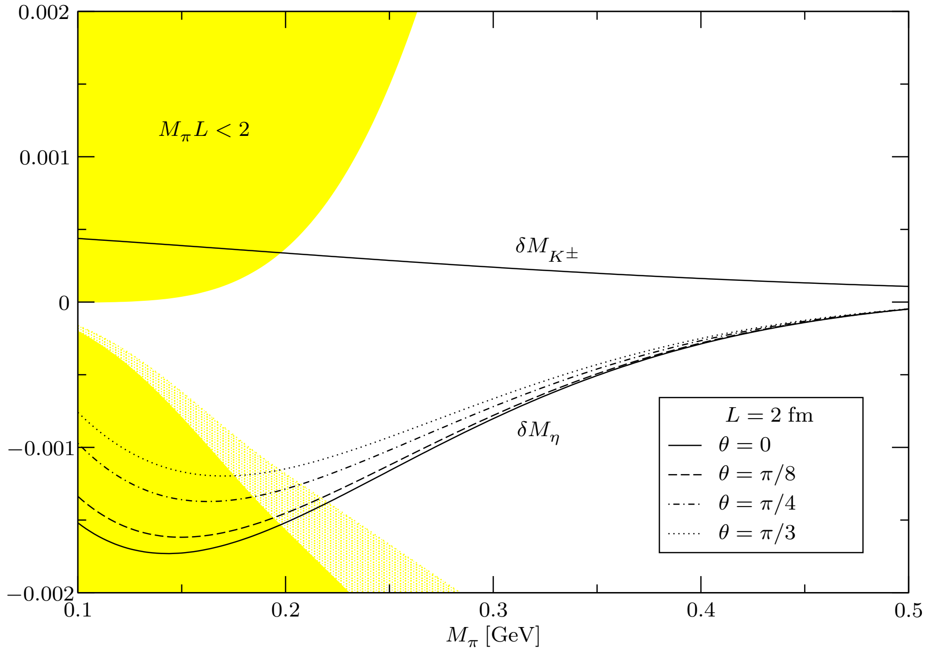


(a) Pion mass dependence of δM_{π^0}.

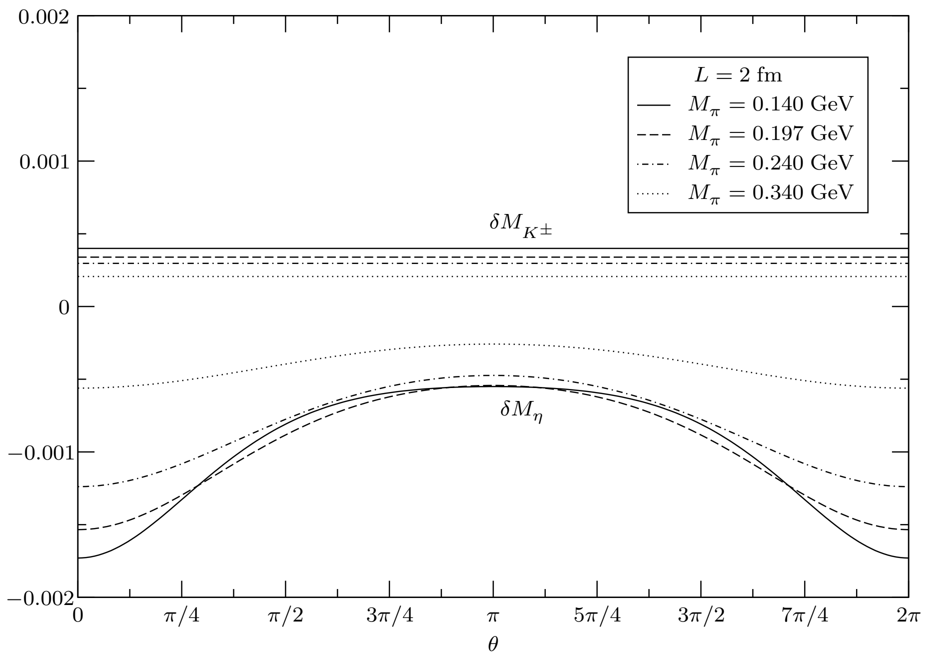


(b) Angle dependence of δM_{π^0}.

Figure 5.4: Mass corrections of the neutral pion at NLO. Note that in (a) $\delta M_{\pi^\pm}$ is given by the solid lines ($\theta = 0$) whereas in (b) it would be constant and would value as δM_{π^0} at $\theta = 0$.



(a) Pion mass dependence of $\delta M_{K^\pm}$, δM_η.



(b) Angle dependence of $\delta M_{K^\pm}$, δM_η.

Figure 5.5: Mass corrections of charged kaons and eta meson at NLO.

This is a negligible effect.

Renormalization Terms

In Fig. 5.6—5.8 we represent the dependences on M_π and on θ of the renormalization terms $\Delta\vartheta^\mu_{\pi^+}$, $\Delta\vartheta^\mu_{K^+}$, $\Delta\vartheta^\mu_{K^0}$. We represent the first component (i.e. $\mu = 1$) as for the configuration (5.7) it is the only one which is non-zero. Since $\Delta\vartheta^\mu_{\pi^+}$, $\Delta\vartheta^\mu_{K^+}$, $\Delta\vartheta^\mu_{K^0}$ are dimensionful quantities, the values on the y-axis are in given in GeV. We remind the reader that renormalization terms are here not treated as parts of corrections. However, they should be then taken into account when extrapolating physical observables from lattice simulations as they enter the expressions of energies and matrix elements.

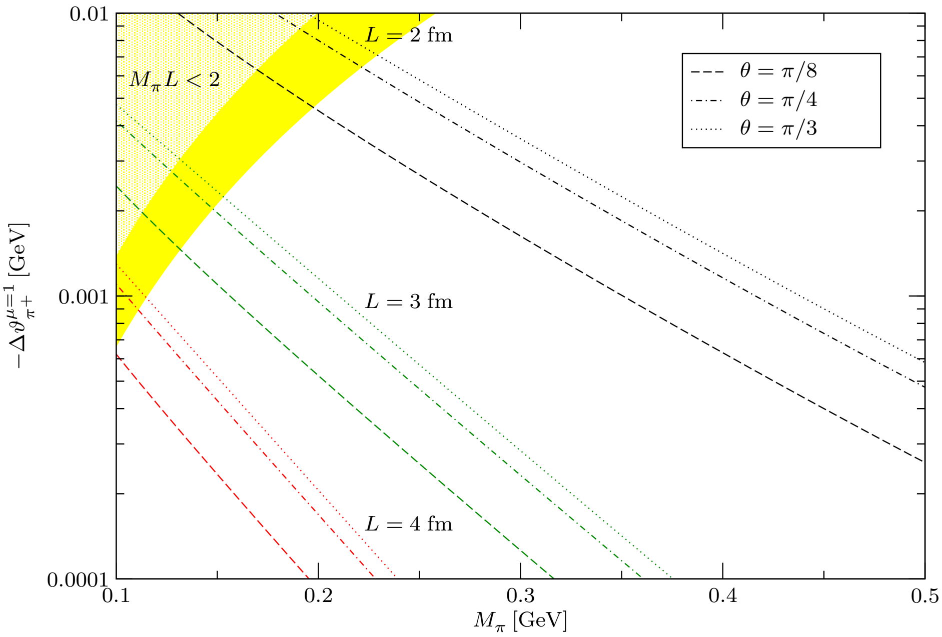
In Fig. 5.6a we represent the pion mass dependence of $-\Delta\vartheta^\mu_{\pi^+}$ whereas in Fig. 5.7a (resp. Fig. 5.8a) we represent the pion mass dependence of $-\Delta\vartheta^\mu_{K^+}$ (resp. $\Delta\vartheta^\mu_{K^0}$). The logarithmic graphs well illustrate the exponential decay in M_π. The renormalization terms decay as $\mathcal{O}(\mathrm{e}^{-M_\pi L})$ and are represent by straight lines. The slopes depend on the values of L while the y-intercepts on the value of θ. Note that for $\theta \in \{\,0,\, \pi/8,\, \pi/4,\, \pi/3\,\}$ the absolute values of the renormalization terms increase with the angle. If we take a fixed angle, then $-\Delta\vartheta^\mu_{\pi^+}$ is bigger than $-\Delta\vartheta^\mu_{K^+}$, $\Delta\vartheta^\mu_{K^0}$. The reason is that the contribution of virtual pions in $-\Delta\vartheta^\mu_{\pi^+}$ is a factor 2 bigger than those in $-\Delta\vartheta^\mu_{K^+}$, $\Delta\vartheta^\mu_{K^0}$, see Eqs. (2.31, 2.41).

In Fig. 5.6b we represent the angle dependence of $\Delta\vartheta^\mu_{\pi^+}$ and in Fig. 5.7b (resp. Fig. 5.8b) that of $\Delta\vartheta^\mu_{K^+}$ (resp. $\Delta\vartheta^\mu_{K^0}$). We observe that the renormalization terms depend on θ nearly as sinus functions. The zeros correspond to integer multiples of π and the extrema (i.e. minima and maxima) are close to half-integer multiples of π. In this case, the slight displacement of extrema is due to the specific form of the function $\mathrm{f}^\mu_1(\lambda_P, \vartheta)$, see Eq. (2.33).

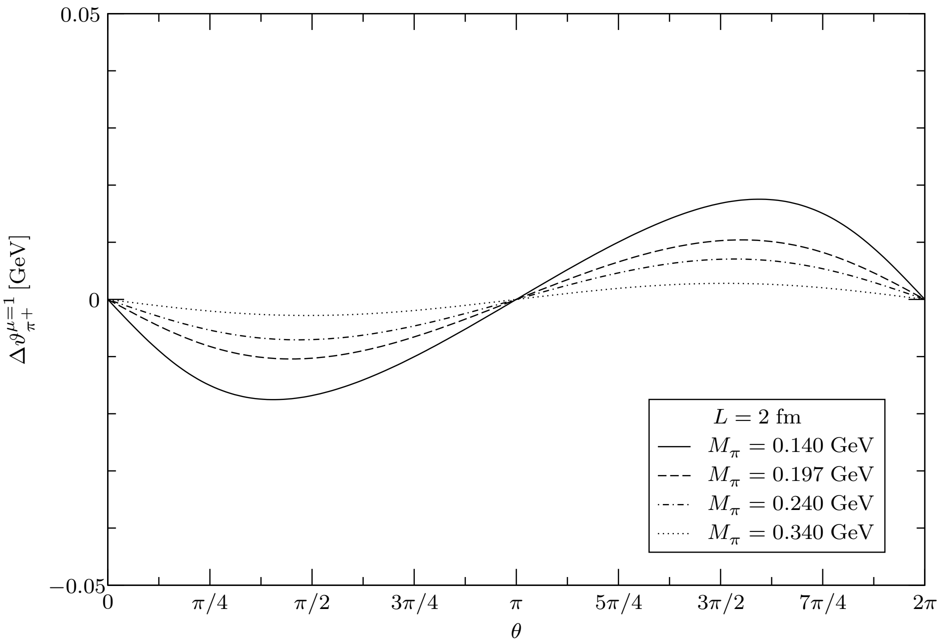
5.2.2 Decay Constants

At NLO the corrections of the decay constants exhibit all a dependence on twisting angles. However, δF_{K^0} can be determined from $\delta F_{K^\pm}$ substituting $\vartheta_{K^0} \leftrightarrow \vartheta_{K^+}$ in Eqs. (2.54c, 2.54d) and on their own, δF_{π^0}, δF_η are of no phenomenological interest. We then concentrate on $\delta F_{\pi^\pm}$, $\delta F_{K^\pm}$ in our numerical analysis.

In Fig. 5.9a (resp. Fig. 5.10a) we represent the pion mass dependence of $-\delta F_{\pi^\pm}$ (resp. $-\delta F_{K^\pm}$). The logarithmic graphs illustrate the exponential decay $\mathcal{O}(\mathrm{e}^{-M_\pi L})$ of the corrections. In general, the corrections are negative and for $\theta \in \{\,0,\, \pi/8,\, \pi/4,\, \pi/3\,\}$ their absolute values decrease with the angle. If we consider $L = 2$ fm, we read that $-\delta F_{\pi^\pm}$ is about 8.6% for $\theta = 0$ (resp. 7.3% for $\theta = \pi/3$) at $M_\pi \approx 0.2$ GeV and decreases to 0.3% at $M_\pi \approx 0.5$ GeV. Considering the same side length, $-\delta F_{K^\pm}$ is about 3.5% for $\theta = 0$ (resp. 2.8% for $\theta = \pi/3$) at $M_\pi \approx 0.2$ GeV and decreases to 0.2% at $M_\pi \approx 0.5$ GeV. Such corrections can be comparable with the statistical precision of lattice simulations. In Section 5.4 we will see that $\delta F_{\pi^\pm}$, $\delta F_{K^\pm}$ are sometimes understimated by lattice practitioners whereas they may be sizable effects. From Fig. 5.9a and Fig. 5.10a we also observe that the corrections of the decay constant are bigger –in absolute value– than the mass correc-

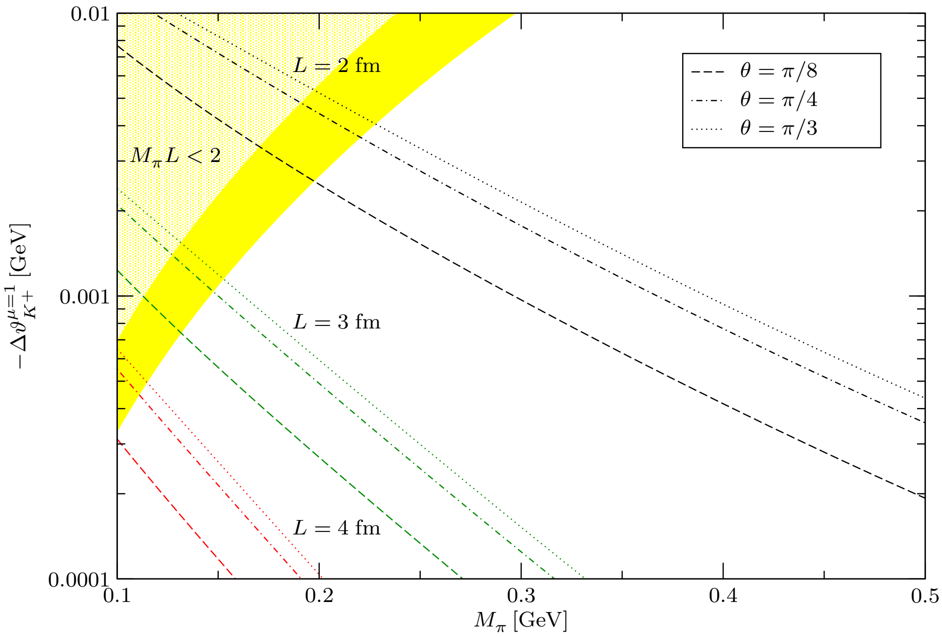


(a) *Pion mass dependence of* $-\Delta\vartheta^{\mu}_{\pi^+}$ *for* $\mu = 1$.

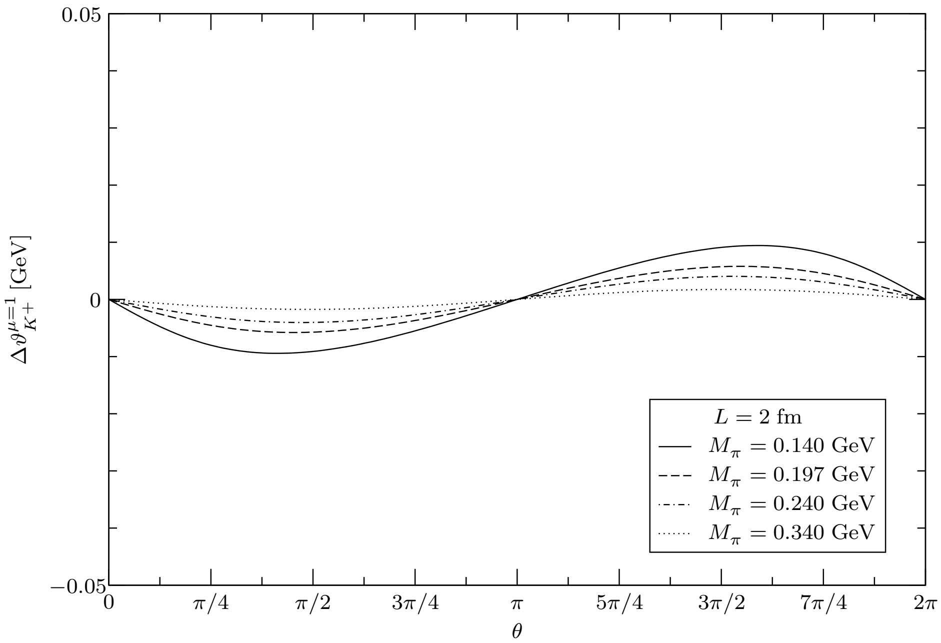


(b) *Angle dependence of* $\Delta\vartheta^{\mu}_{\pi^+}$ *for* $\mu = 1$.

Figure 5.6: Renormalization terms of charged pions at NLO. Note that in (a) the dark yellow area refers to the region $M_\pi L < 2$ *for* $\theta = \pi/8$.

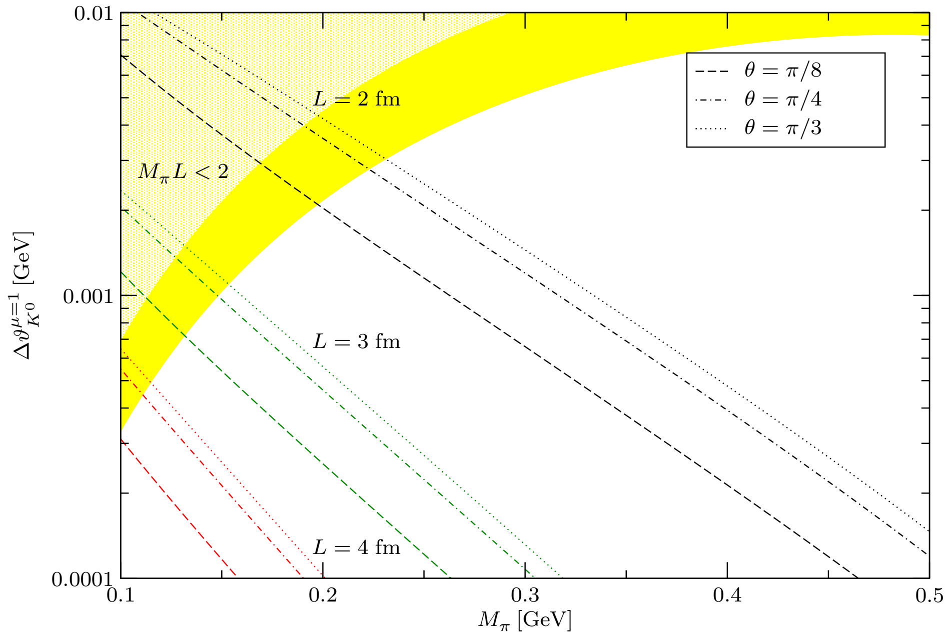


(a) Pion mass dependence of $-\Delta\vartheta^{\mu}_{K^+}$ for $\mu = 1$.

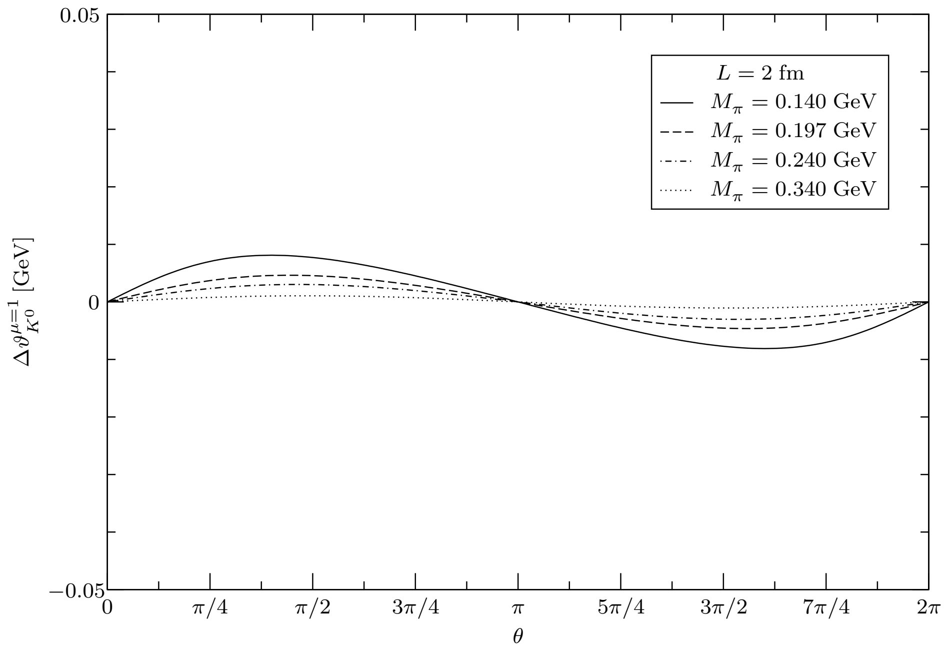


(b) Angle dependence of $\Delta\vartheta^{\mu}_{K^+}$ for $\mu = 1$.

Figure 5.7: Renormalization terms of charged kaons at NLO. Note that in (a) the dark yellow area refers to the region $M_\pi L < 2$ for $\theta = \pi/8$.



(a) Pion mass dependence of $\Delta\vartheta^{\mu}_{K^0}$ for $\mu = 1$.



(b) Angle dependence of $\Delta\vartheta^{\mu}_{K^0}$ for $\mu = 1$.

Figure 5.8: Renormalization terms of the neutral kaon at NLO. Note that in (a) the dark yellow area refers to the region $M_\pi L < 2$ for $\theta = \pi/8$.

tions. This can be explained comparing the expressions (2.54) with those of Eq. (2.43). In $-\delta F_{\pi^\pm}$ (resp. $-\delta F_{K^\pm}$) the contribution of virtual pions is bigger than that of $\delta M_{\pi^\pm}$ (resp. $\delta M_{K^\pm}$). Since the contribution of virtual pions is dominant, the corrections of the decay constant are bigger than those of masses. As a side remark we note that $-\delta F_{K^\pm}$ is smaller than $-\delta F_{\pi^\pm}$ because of a prefactor 3/8 suppressing the contribution of virtual pions in the expression of charged kaons, see Eqs. (2.54b, 2.54c).

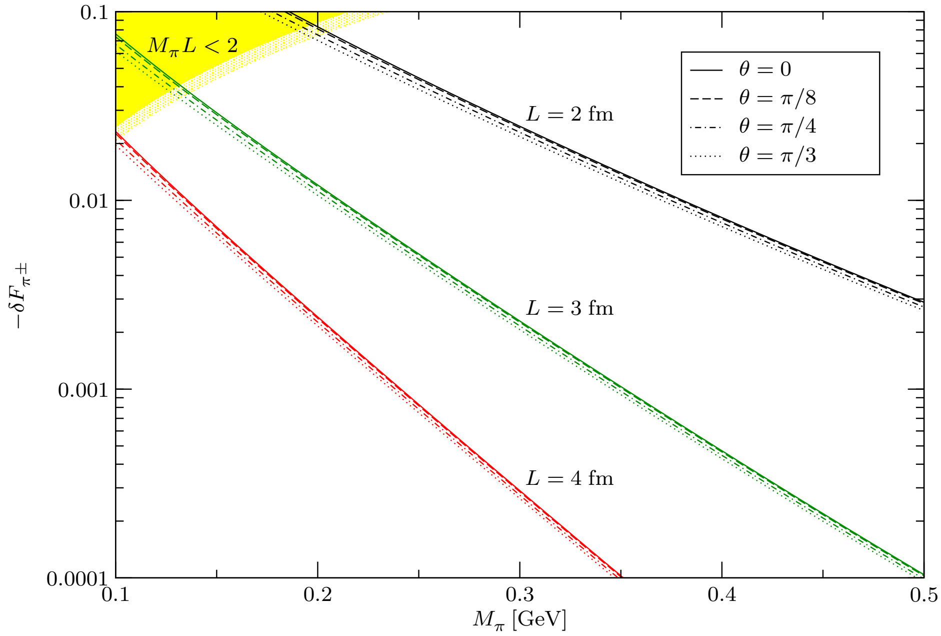
In Fig. 5.9b (resp. Fig. 5.10b) we represent the angle dependence of $\delta F_{\pi^\pm}$ (resp. $\delta F_{K^\pm}$). We observe that the corrections depend on θ as negative cosinus functions. The maxima (resp. minima) are located at odd (resp. even) integer multiples of π. If we consider $M_\pi = 0.197$ GeV, the difference among maxima and minima is 4.0% in $\delta F_{\pi^\pm}$ (resp. 2.1% in $\delta F_{K^\pm}$) at $L = 2$ fm. These are sizable effects and should be taken into account when physical observables are extrapolated from lattice data at different twisting angles.

5.2.3 Pseudoscalar Coupling Constants

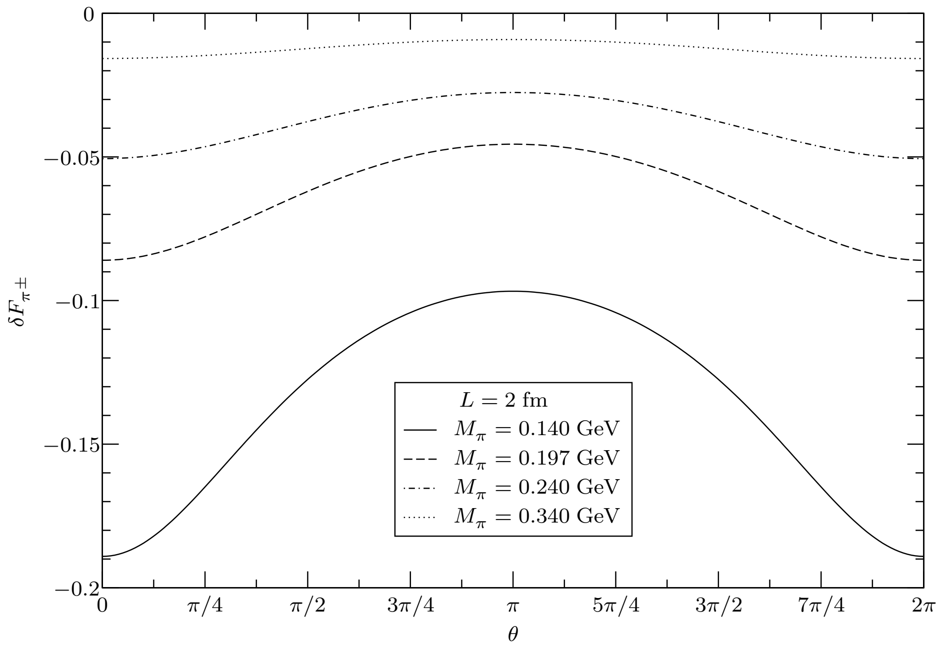
At NLO the corrections of the pseudoscalar coupling constants exhibit all a dependence on twisting angles. In Section 2.3.3 we have seen that the corrections of the pseudoscalar coupling constants are related to those of masses and decay constants. The relations originate from chiral Ward identities and allow one to determine the corrections of pseudoscalar coupling constants from the sum of the mass corrections plus the corrections of decay constants, see Eqs. (2.67, 2.68). Since we have numerically estimated $\delta M_{\pi^\pm}$, $\delta M_{K^\pm}$ and $\delta F_{\pi^\pm}$, $\delta F_{K^\pm}$ we can determine $\delta G_{\pi^\pm}$, $\delta G_{K^\pm}$ by means of such relations. Moreover, δG_{K^0} can be determined from $\delta G_{K^\pm}$ substituting $\vartheta_{K^0} \leftrightarrow \vartheta_{K^+}$ in Eqs. (2.58c, 2.58d). Therefore, we concentrate on δG_{π^0}, δG_η which must be numerically evaluated from Eqs. (2.58a, 2.58e).

In Fig. 5.11a (resp. Fig. 5.12a) we represent the pion mass dependence of $-\delta G_{\pi^0}$ (resp. $-\delta G_\eta$). The logarithmic graphs illustrate the exponential decay $\mathcal{O}(\mathrm{e}^{-M_\pi L})$ of the corrections. In Fig. 5.11a the lines are so close that they overlap in the graph. On the contrary, the lines of Fig. 5.12a are distinguishable for different angles. In general, the corrections are negative and for $\theta \in \{\,0,\ \pi/8,\ \pi/4,\ \pi/3\,\}$ their absolute values decrease with the angle. If we consider $L = 2$ fm, we read that $-\delta G_{\pi^0}$ is about 4.4% at $M_\pi \approx 0.2$ GeV and decreases to 0.2% at $M_\pi \approx 0.5$ GeV. Considering the same side length, $-\delta G_\eta$ is about 4.4% for $\theta = 0$ (resp. 3.5% for $\theta = \pi/3$) at $M_\pi \approx 0.2$ GeV and decreases to 0.2% at $M_\pi \approx 0.5$ GeV. From these values, we observe that $-\delta G_{\pi^0} \approx -\delta G_\eta$ for $\theta = 0$. This can be understood if we look the expressions of the corrections at NLO for vanishing twisting angles, see Eq. (2.73). In that case, the contribution of virtual pions in δG_{π^0} and in δG_η are equal. As this is the dominant contribution, we conclude that for $\theta = 0$ the corrections are similar, namely $-\delta G_{\pi^0} \approx -\delta G_\eta$.

In Fig. 5.11b we represent the angle dependence of δG_{π^0}. We observe that δG_{π^0} is practically constant for the configuration (5.7). This is explicable as at NLO the contribution of virtual pions in δG_{π^0} does not depend on twisting angles, see Eq. (2.58a). The angle dependence is due to the contribution of virtual kaons which is however suppressed as $\mathcal{O}(\mathrm{e}^{-M_K L})$. In principle, δG_{π^0} depends on θ as a negative cosinus but the cosinus is so suppressed that δG_{π^0} results almost constant. In Fig. 5.12b we represent the angle

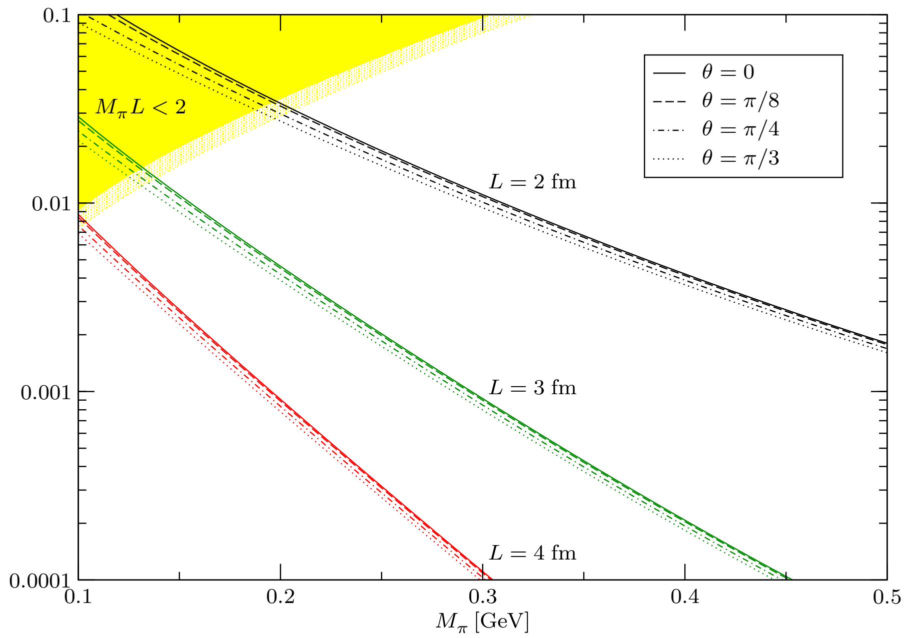


(a) Pion mass dependence of $-\delta F_{\pi^\pm}$*.*

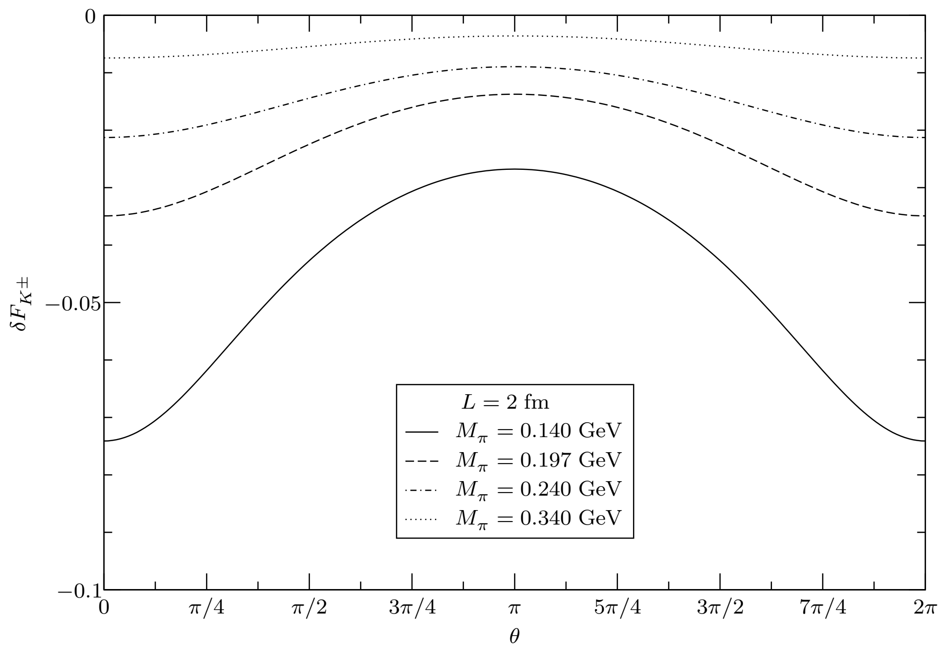


(b) Angle dependence of $\delta F_{\pi^\pm}$*.*

Figure 5.9: Corrections of the decay constants of charged pions at NLO.

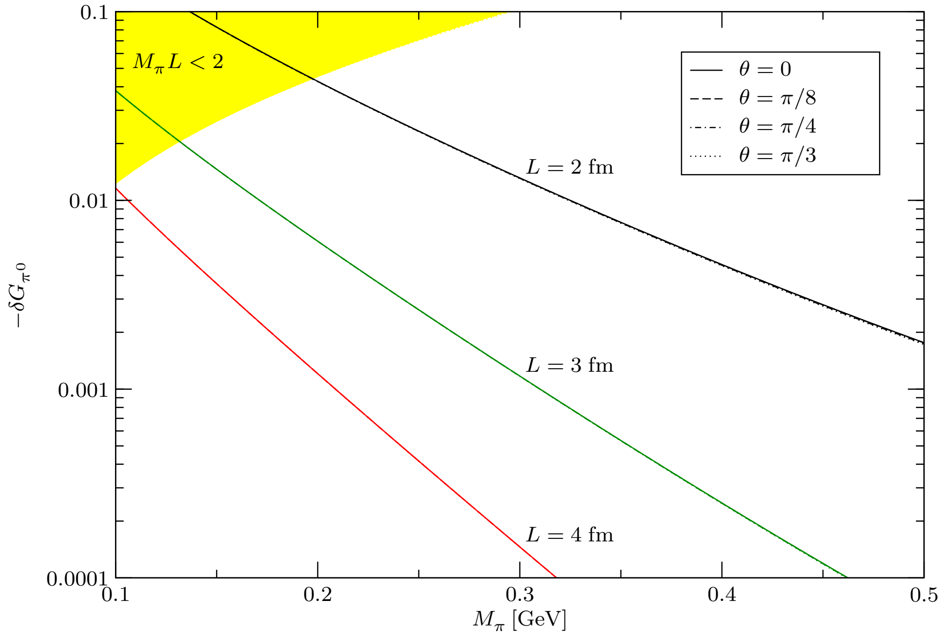


(a) *Pion mass dependence of* $-\delta F_{K^\pm}$.

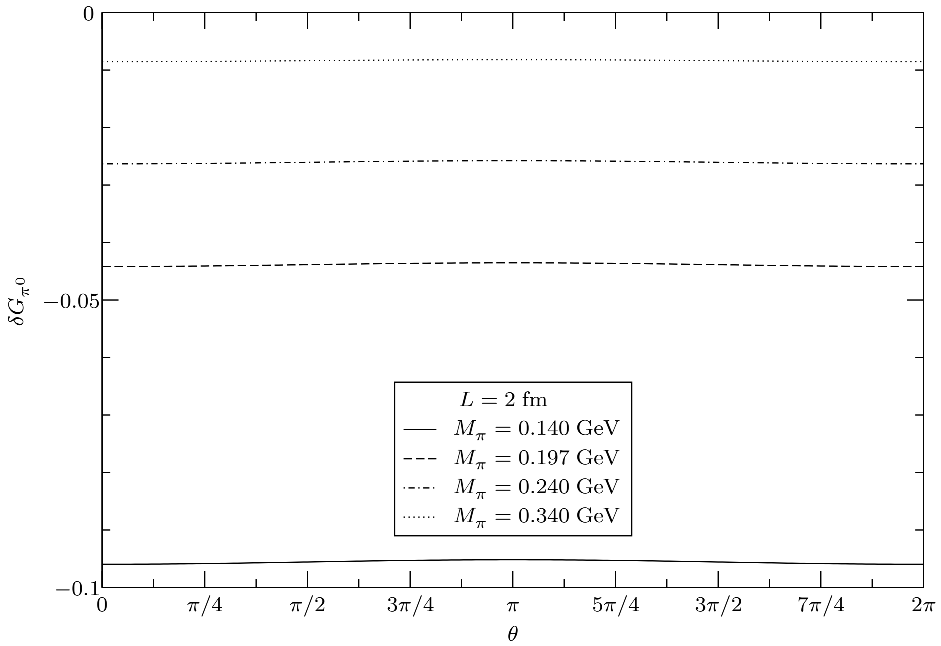


(b) *Angle dependence of* $\delta F_{K^\pm}$.

Figure 5.10: Corrections of the decay constants of charged kaons at NLO.

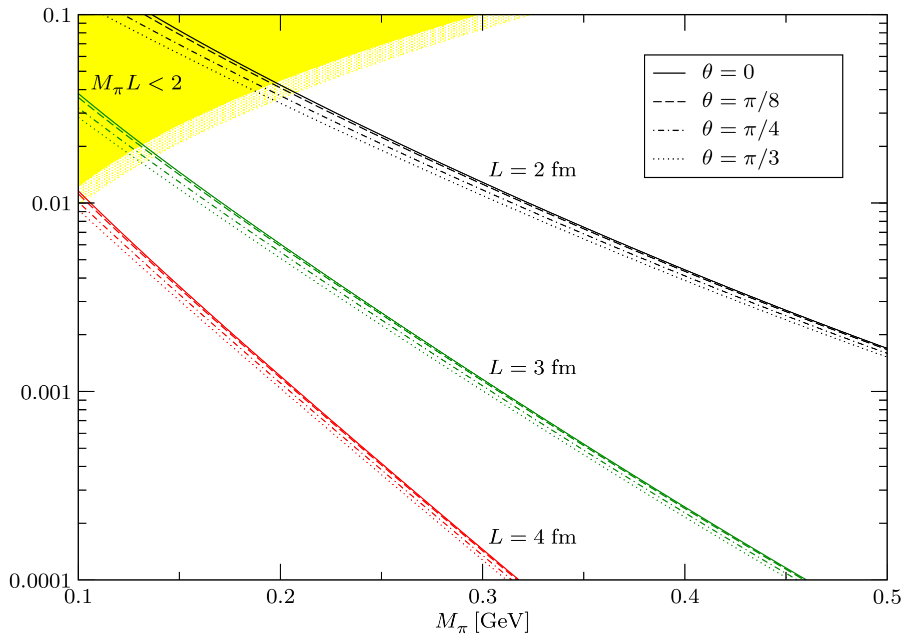


(a) Pion mass dependence of $-\delta G_{\pi^0}$.

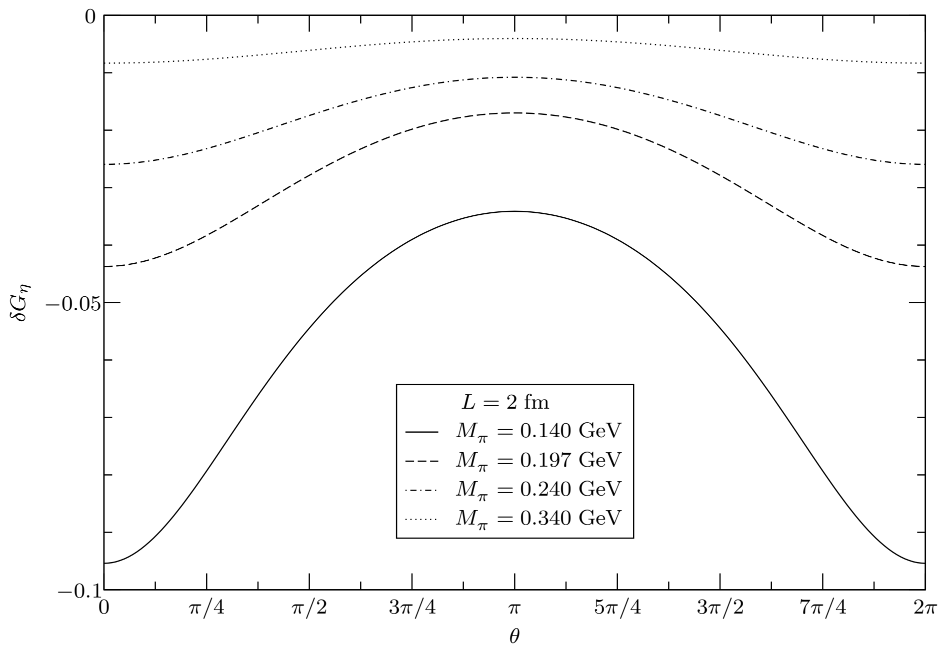


(b) Angle dependence of δG_{π^0}.

Figure 5.11: Corrections of the pseudoscalar coupling constant of the neutral pion at NLO.



(a) Pion mass dependence of $-\delta G_\eta$.



(b) Angle dependence of δG_η.

Figure 5.12: Corrections of the coupling constant of the eta meson at NLO.

dependence of δG_η. We observe that δG_η depends on θ as a negative cosinus function. The maxima (resp. minima) are located at odd (resp. even) integer multiples of π. If we consider $M_\pi = 0.197$ GeV, the difference among maxima and minima is 2.7% at $L = 2$ fm. Most of this difference is due to the contribution of virtual charged pions.

5.2.4 Pion Form Factors

Vanishing Momentum Transfer

We consider pions at rest and estimate the corrections of the matrix elements of form factors at a vanishing momentum transfer (i.e. $q^2 = 0$). Here, we concentrate on $\delta\Gamma_S^{\pi^0}$, $\delta\Gamma_S^{\pi^+}$, $(\Delta\Gamma_V^{\pi^+})^\mu$ and represent their dependences on M_π and on θ.

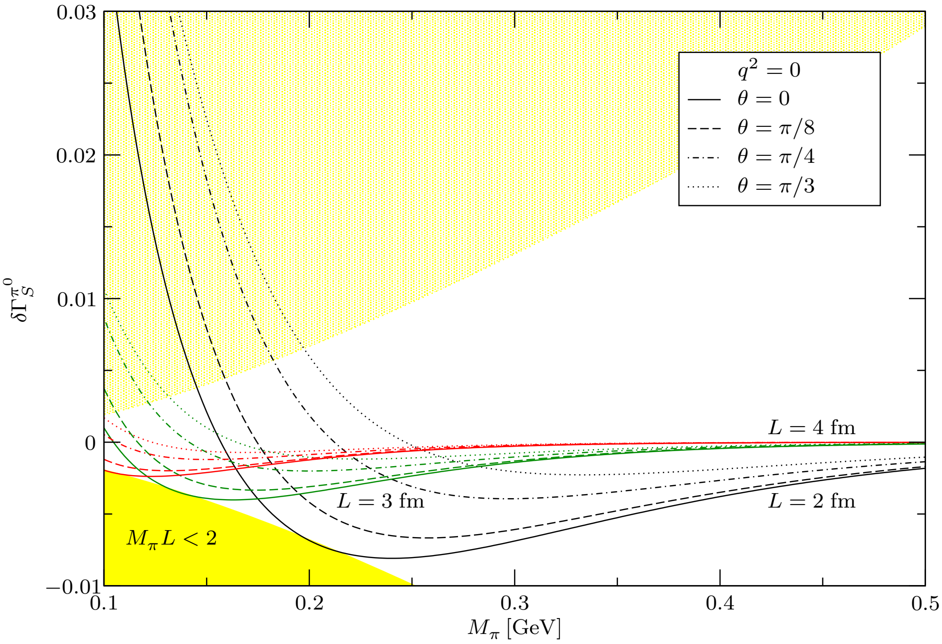
In Fig. 5.13a (resp. Fig. 5.14a) we represent the pion mass dependence of $\delta\Gamma_S^{\pi^0}$ (resp. $\delta\Gamma_S^{\pi^+}$) at $q^2 = 0$. The yellow areas refer to the region $M_\pi L < 2$. The solid lines ($\theta = 0$) reach that region when –starting from the right-hand side of the figure– they first touch the dark yellow area. The dotted lines ($\theta = \pi/3$) reach this region when they enter in the light yellow area. We remind the reader that for $M_\pi L < 2$ the p-regime is not guaranteed and numerical results should be taken with a grain of salt.

From the graphs, we observe that the corrections decay exponentially as $\mathcal{O}(\mathrm{e}^{-M_\pi L})$ and they are mainly negative. The corrections may turn positive depending on the pion mass. If we consider $L = 2$ fm, we read that $\delta\Gamma_S^{\pi^0}$ is about -0.7% for $\theta = 0$ (resp. 0.6% for $\theta = \pi/3$) at $M_\pi \approx 0.2$ GeV and amounts to -0.2% for $\theta = 0$ (resp. -0.1% for $\theta = \pi/3$) at $M_\pi \approx 0.5$ GeV. Considering the same side length, $\delta\Gamma_S^{\pi^+}$ is about -0.7% for $\theta = 0$ (resp. 3.5% for $\theta = \pi/3$) at $M_\pi \approx 0.2$ GeV and amounts to -0.2% for $\theta = 0$ (resp. -0.1% for $\theta = \pi/3$) at $M_\pi \approx 0.5$ GeV. Note that for $\theta = 0$ the corrections $\delta\Gamma_S^{\pi^0}$, $\delta\Gamma_S^{\pi^+}$ are equal as expected in the case of PBC.

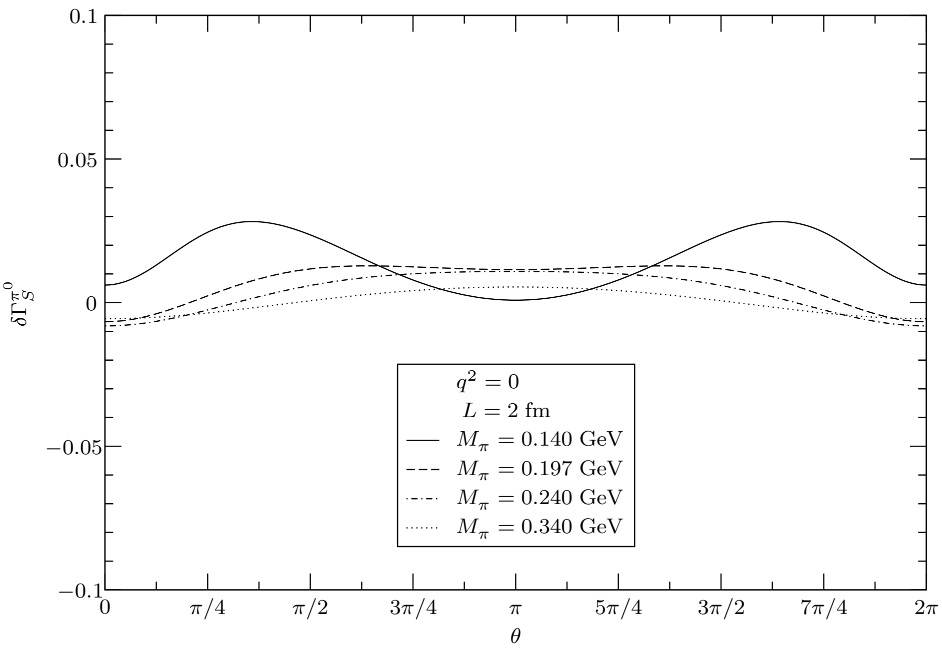
In Fig. 5.13b we represent the angle dependence of $\delta\Gamma_S^{\pi^0}$ at $q^2 = 0$. We observe that $\delta\Gamma_S^{\pi^0}$ depends on θ nearly as a negative cosinus function. The shape is deformed due to the cancellation among the functions $\mathrm{g}_1(\lambda_P, \vartheta)$, $\mathrm{g}_2(\lambda_P, \vartheta)$, see Eq. (2.86a). In Fig. 5.14b is represented the angle dependence of $\delta\Gamma_S^{\pi^+}$ at $q^2 = 0$. We observe that $\delta\Gamma_S^{\pi^+}$ depends on θ nearly as $\theta \sin\theta$. Such dependence originates from the last term of Eq. (2.86b) and provides large corrections for large angles. To minimize the corrections it is then important to employ small angles, i.e. $\theta < \pi$.

The corrections of the matrix elements of the vector form factor are represented in Fig. 5.15. We represent the first component as for the configuration (5.7) it is the only one which is non-zero. Since $(\Delta\Gamma_V^{\pi^+})^\mu$ is dimensionful, the values on the y-axis are given in GeV.

In Fig. 5.15a we represent the pion mass dependence of $-(\Delta\Gamma_V^{\pi^+})^\mu$ at $q^2 = 0$. The logarithmic graph illustrates that the corrections decay exponentially as $\mathcal{O}(\mathrm{e}^{-M_\pi L})$. They are mainly negative and for $\theta \in \{0, \pi/8, \pi/4, \pi/3\}$ their absolute value increases with the angle. Note that the corrections disappear for $\theta = 0$. This because we are considering the case of pions at rest (i.e. $\vec{p} = \vec{0}$) for which the corrections (2.96) disappear when $\vartheta^\mu_{\pi^\pm} = 0$. In Fig. 5.15b is represented the angle dependence of $(\Delta\Gamma_V^{\pi^+})^\mu$ at $q^2 = 0$. We observe that

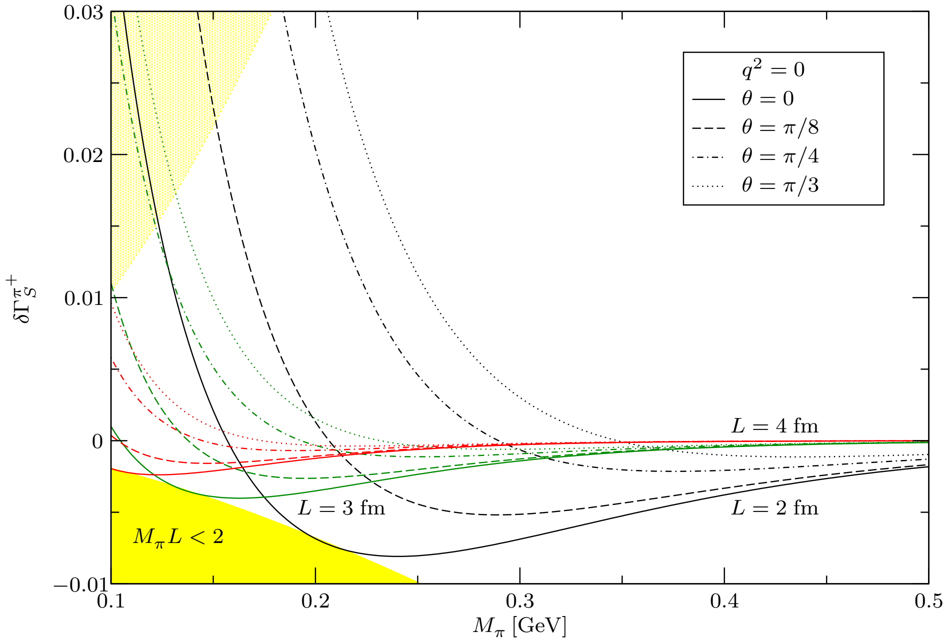


(a) Pion mass dependence of $\delta\Gamma_S^{\pi^0}$ at $q^2 = 0$.

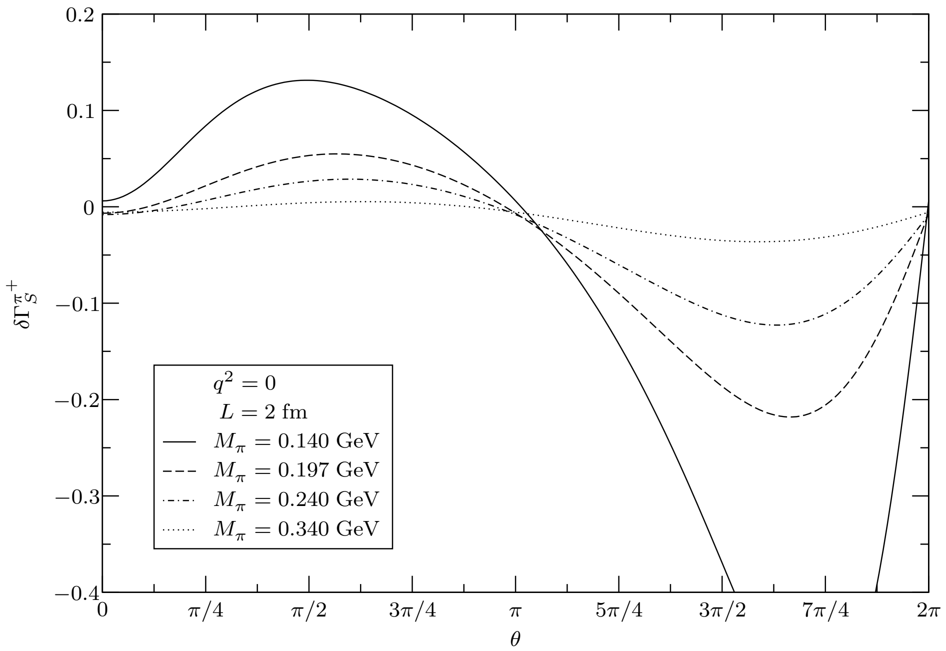


(b) Angle dependence of $\delta\Gamma_S^{\pi^0}$ at $q^2 = 0$.

Figure 5.13: Corrections of the matrix element of the scalar form factor at NLO.

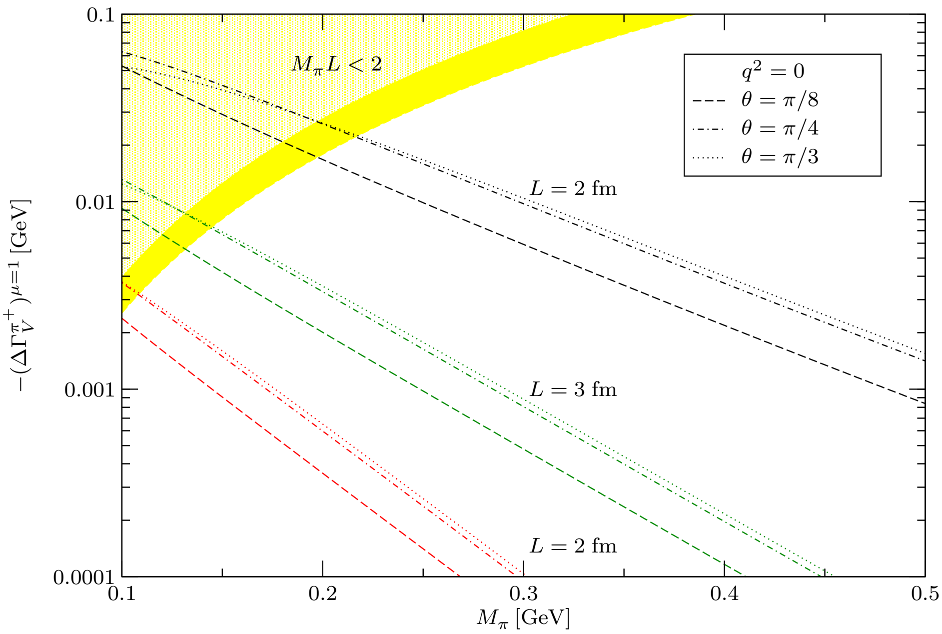


(a) *Pion mass dependence of* $\delta\Gamma_S^{\pi^+}$ *at* $q^2 = 0$.

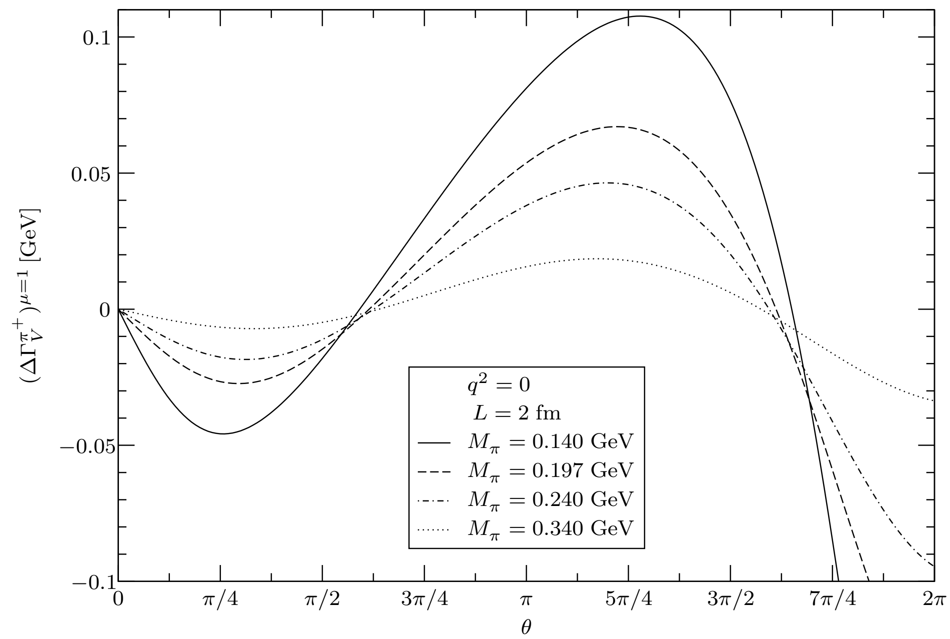


(b) *Angle dependence of* $\delta\Gamma_S^{\pi^+}$ *at* $q^2 = 0$.

Figure 5.14: Corrections of the matrix element of the scalar form factor at NLO.



(a) Pion dependence of $-(\Delta\Gamma_V^{\pi^+})^\mu$ for $\mu = 1$ at $q^2 = 0$.



(b) Angle dependence of $(\Delta\Gamma_V^{\pi^+})^\mu$ for $\mu = 1$ at $q^2 = 0$.

Figure 5.15: Corrections of the matrix element of the vector form factor at NLO. Note that in (a) the dark yellow area refers to the region $M_\pi L < 2$ for $\theta = \pi/8$.

$(\Delta\Gamma_V^{\pi^+})^\mu$ depends on θ nearly as $-(\theta\cos\theta+\sin\theta)$. The enhanced cosinus dependence (i.e. $-\theta\cos\theta$) originates from the contraction of the external twisting angle with the function $\mathrm{h}_2^{\mu\nu}(\lambda_P,\vartheta)$. This provides large corrections for large angles. The sinus dependence $(-\sin\theta)$ originates from the renormalization term $\Delta\vartheta^\mu_{\pi^+}$ as already observed in Section 5.2.1.

Non-zero Momentum Transfer

To estimate the corrections at a non-zero momentum transfer we consider the incoming pion at rest (i.e. $\vec{p}=\vec{0}$) and the outgoing pion moving along the first axis carrying the first non-zero momentum (i.e. $|\vec{p}\,'|=2\pi/L$). This kinematics provides the minimal momentum transfer,

$$q^\mu_{\min}=\begin{pmatrix}q^0\\ \vec{q}\end{pmatrix}\qquad\text{with}\qquad \vec{q}=\frac{2\pi}{L}\begin{pmatrix}1\\0\\0\end{pmatrix}. \tag{5.9}$$

The zeroth component corresponds to the energy transfer among external pions,

$$\begin{aligned} q^0 &= E'_{\pi^0}(L)-M_{\pi^0}(L) \quad \text{for external } \pi^0,\\ q^0 &= E'_{\pi^+}(L)-E_{\pi^+}(L) \quad \text{for external } \pi^+. \end{aligned} \tag{5.10}$$

For the configuration (5.7) the pion energies take the following forms,

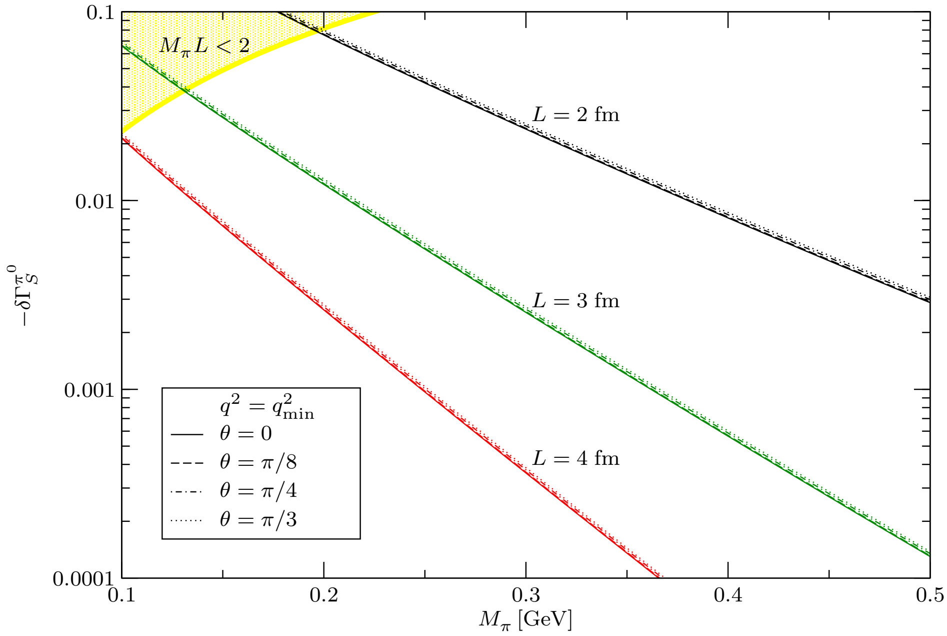
$$\begin{aligned} E'_{\pi^0}(L) &= \sqrt{M^2_{\pi^0}(L)+(2\pi)^2/L^2}\\ E_{\pi^+}(L) &= \sqrt{M^2_{\pi^\pm}(L)+(\theta/L)^2+2\,\theta\Delta\vartheta/L+\mathcal{O}(\xi_\pi^2)}\\ E'_{\pi^+}(L) &= \sqrt{M^2_{\pi^\pm}(L)+(2\pi+\theta)^2/L^2+2\,(2\pi+\theta)\Delta\vartheta/L+\mathcal{O}(\xi_\pi^2)}. \end{aligned} \tag{5.11}$$

Here, $M_{\pi^0}(L)$, $M_{\pi^\pm}(L)$ are the pion masses in finite volume and their corrections are given in Eq. (2.75a) in the case of 2-light-flavor ChPT. The quantity,

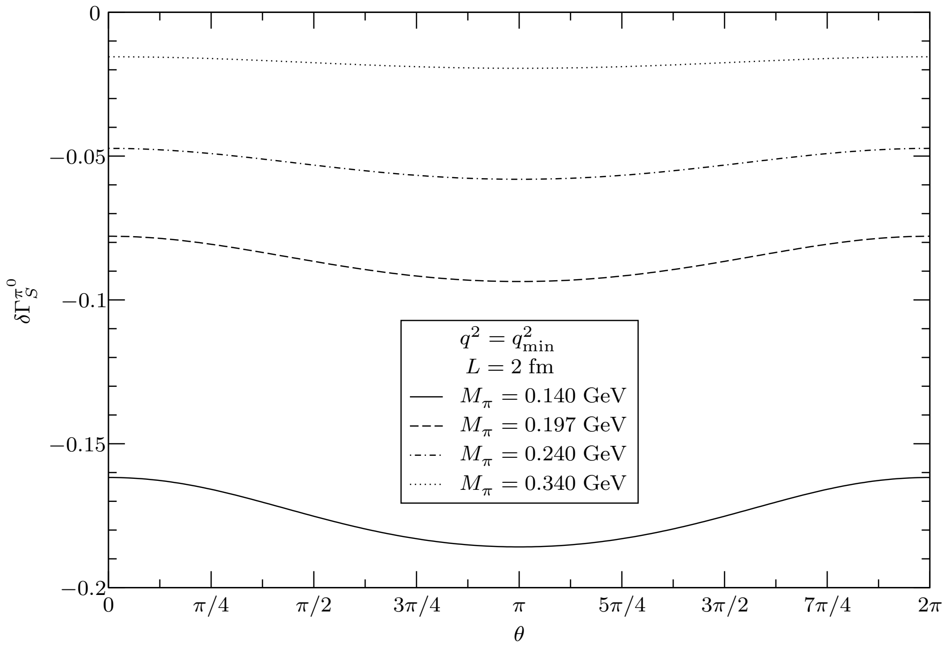
$$\Delta\vartheta=\xi_\pi\sum_{n=1}^{\infty}\frac{4i}{Ln}\,K_2(\lambda_\pi\sqrt{n})\sum_{n_1=-\lfloor\sqrt{n}\rfloor}^{\lfloor\sqrt{n}\rfloor} m(n,n_1)\,n_1\mathrm{e}^{in_1\theta}, \tag{5.12}$$

corresponds to the first component of the renormalization term (2.76) evaluated for the configuration (5.7).

In Fig. 5.16a (resp. Fig. 5.17a) we represent the pion mass dependence of $-\delta\Gamma_S^{\pi^0}$ (resp. $-\delta\Gamma_S^{\pi^+}$) at $q^2=q^2_{\min}$. The logarithmic graphs illustrate the exponential decay $\mathcal{O}(\mathrm{e}^{-M_\pi L})$ of the corrections. The corrections are mainly negative. For $\theta\in\{\,0,\ \pi/8,\ \pi/4,\ \pi/3\,\}$ the absolute value of $\delta\Gamma_S^{\pi^0}$ increases (resp. that of $\delta\Gamma_S^{\pi^+}$ decreases) with the angle. If we consider $L=2$ fm, we read that $-\delta\Gamma_S^{\pi^0}$ is about 7.8% for $\theta=0$ (resp. 8.2% for $\theta=\pi/3$) at $M_\pi\approx 0.2$ GeV and decreases to 0.3% at $M_\pi\approx 0.5$ GeV. Considering the same side length, $-\delta\Gamma_S^{\pi^+}$ is about 7.8% for $\theta=0$ (resp. 3.5% for $\theta=\pi/3$) at $M_\pi\approx 0.2$ GeV and decreases to 0.3% for $\theta=0$ (resp. 0.2% for $\theta=\pi/3$) at $M_\pi\approx 0.5$ GeV. From these values we observe

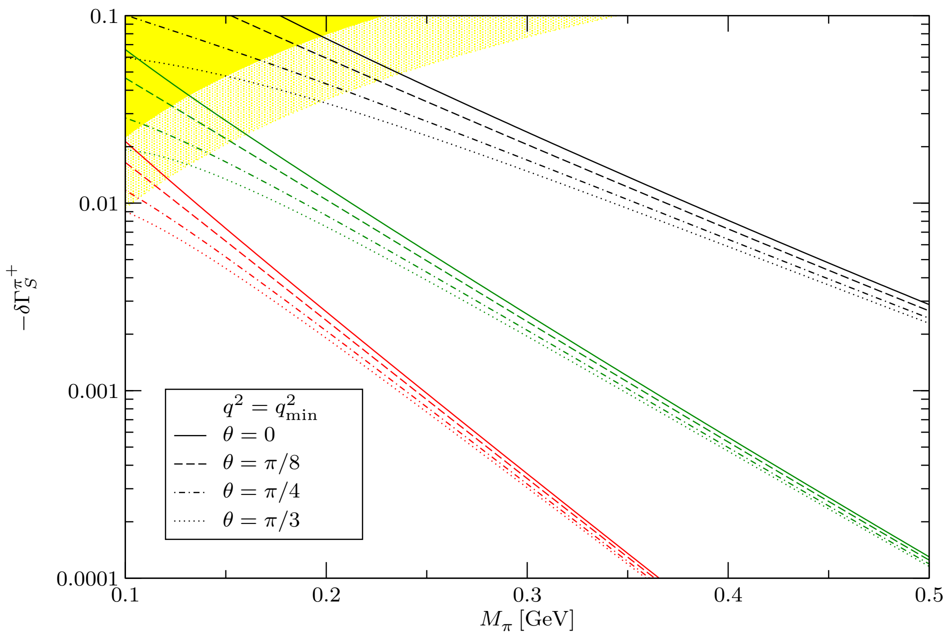


(a) Pion mass dependence of $-\delta\Gamma_S^{\pi^0}$ at $q^2 = q^2_{\rm min}$.

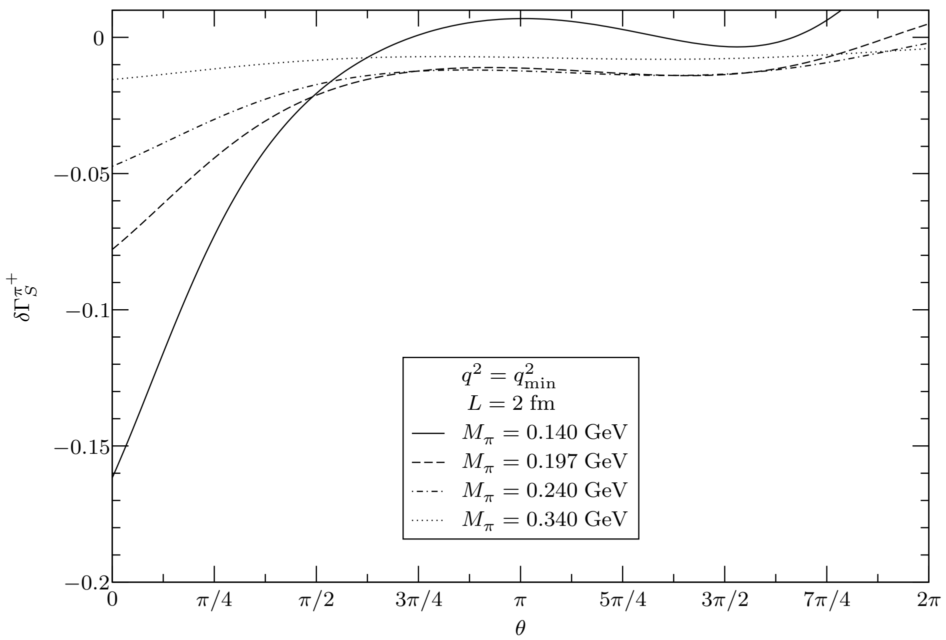


(b) Angle dependence of $\delta\Gamma_S^{\pi^0}$ at $q^2 = q^2_{\rm min}$.

Figure 5.16: Corrections of the matrix element of the scalar form factor at NLO.

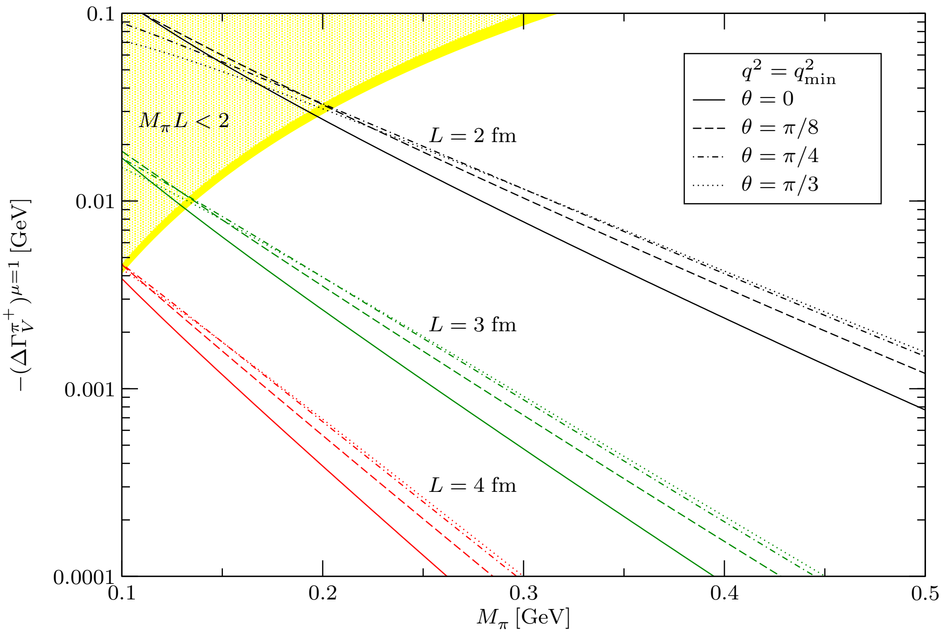


(a) Pion mass dependence of $-\delta\Gamma_S^{\pi^+}$ at $q^2 = q^2_{\min}$.

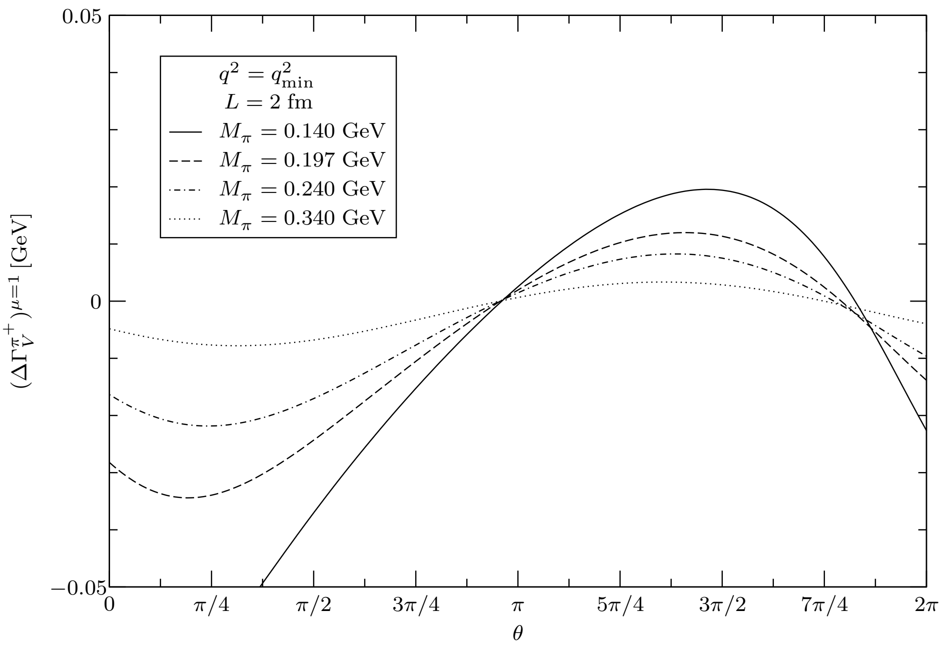


(b) Angle dependence of $\delta\Gamma_S^{\pi^+}$ at $q^2 = q^2_{\min}$.

Figure 5.17: Corrections of the matrix element of the scalar form factor at NLO.

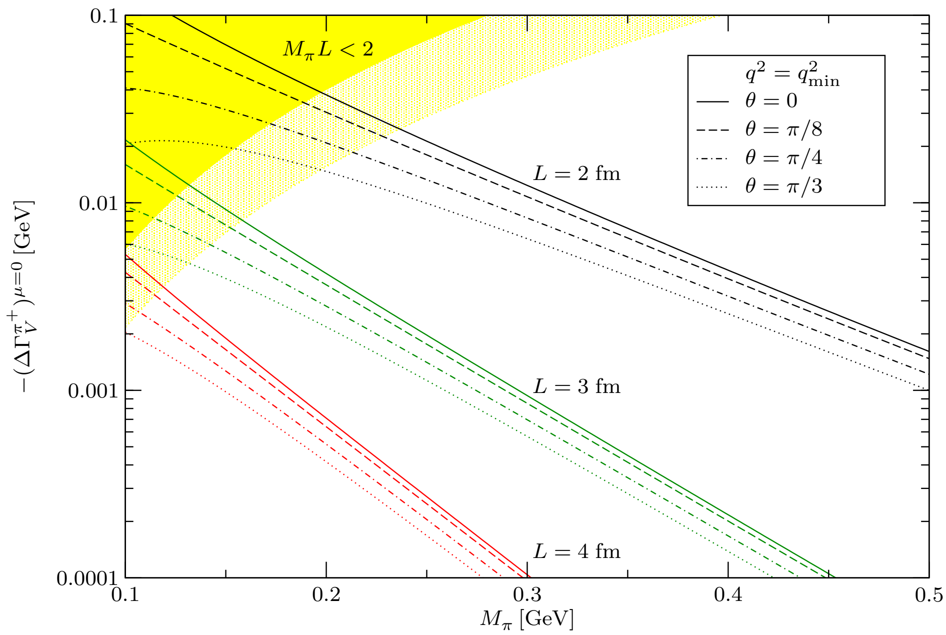


(a) *Pion mass dependence of* $-(\Delta\Gamma_V^{\pi^+})^\mu$ *for* $\mu = 1$ *at* $q^2 = q^2_{\min}$.

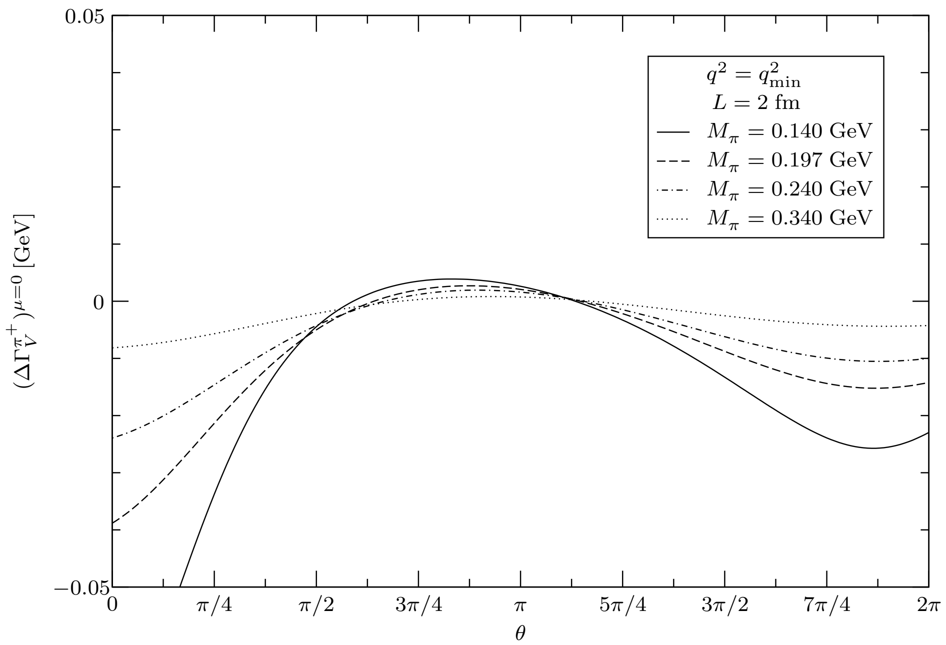


(b) *Angle dependence of* $(\Delta\Gamma_V^{\pi^+})^\mu$ *for* $\mu = 1$ *at* $q^2 = q^2_{\min}$.

Figure 5.18: Corrections of the matrix element of the vector form factor at NLO.



(a) Pion mass dependence of $-(\Delta\Gamma_V^{\pi^+})^\mu$ for $\mu = 0$ at $q^2 = q^2_{\rm min}$.



(b) Angle dependence of $(\Delta\Gamma_V^{\pi^+})^\mu$ for $\mu = 0$ at $q^2 = q^2_{\rm min}$.

Figure 5.19: Corrections of the matrix element of the vector form factor at NLO.

that $\delta\Gamma_S^{\pi^0}$, $\delta\Gamma_S^{\pi^+}$ can be comparable with the statistical precision of lattice simulations. Note also that for $\theta = 0$ the corrections $\delta\Gamma_S^{\pi^0}$, $\delta\Gamma_S^{\pi^+}$ are equal as expected in the case of PBC.

In Fig. 5.16b we represent the angle dependence of $\delta\Gamma_S^{\pi^0}$ at $q^2 = q^2_{\rm min}$. We observe that $\delta\Gamma_S^{\pi^0}$ depends on θ as a cosinus function. The maxima (resp. minima) are located at even (resp. odd) integer multiples of π. If we consider $M_\pi = 0.197$ GeV, the difference among maxima and minima is 1.6% at $L = 2$ fm. This can be sizable effect in very precise lattice simulations and should be taken into account. In Fig. 5.17b is represented the angle dependence of $\delta\Gamma_S^{\pi^+}$ at $q^2 = q^2_{\rm min}$. We observe that $\delta\Gamma_S^{\pi^+}$ depends on θ in a non-trivial way. The dependence mostly originates from the last term of Eq. (2.80b) and provides large corrections for large angles. It is then important to employ small angles (i.e. $\theta < \pi$) to minimize the corrections of the matrix elements.

The corrections of the matrix elements of the vector form factor are represented in Fig. 5.18 and 5.19. We represent the components $\mu = 0, 1$ as they are the only ones which are non-zero for the configuration (5.7). In Fig. 5.18a (resp. Fig. 5.19a) we represent the pion mass dependence of $-(\Delta\Gamma_V^{\pi^+})^\mu$ for $\mu = 1$ (resp. $\mu = 0$). In both cases, the logarithmic graph illustrates the exponential decay $\mathcal{O}(\mathrm{e}^{-M_\pi L})$ of the corrections. The corrections are mainly negative; however, they may turn positive depending on the angle. For $\theta \in \{0,\, \pi/8,\, \pi/4,\, \pi/3\}$ the absolute value of $(\Delta\Gamma_V^{\pi^+})^{\mu=1}$ increases with the angle whereas that of for $(\Delta\Gamma_V^{\pi^+})^{\mu=0}$ is decreasing. In Fig. 5.18b (resp. Fig. 5.19b) we represent the angle dependence of $(\Delta\Gamma_V^{\pi^+})^\mu$ for $\mu = 1$ (resp. $\mu = 0$). We observe that $(\Delta\Gamma_V^{\pi^+})^\mu$ depends on θ in a non-trivial way either for $\mu = 1$ as for $\mu = 0$. These dependences provide large corrections for large angles and it is then important to employ small angles to minimize the corrections.

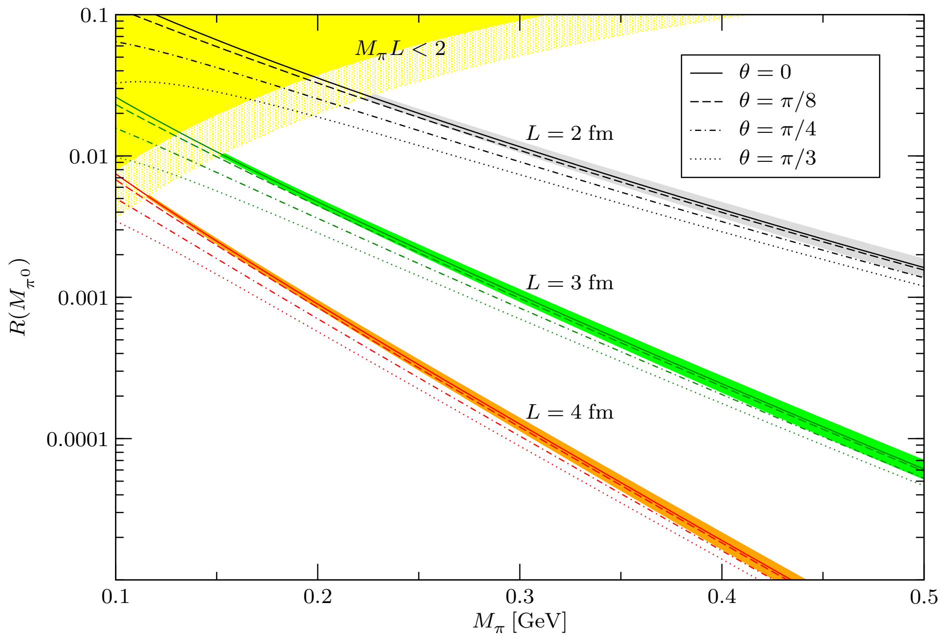
5.3 Finite Volume Corrections beyond NLO

5.3.1 Masses and Renormalization Terms of Self Energies

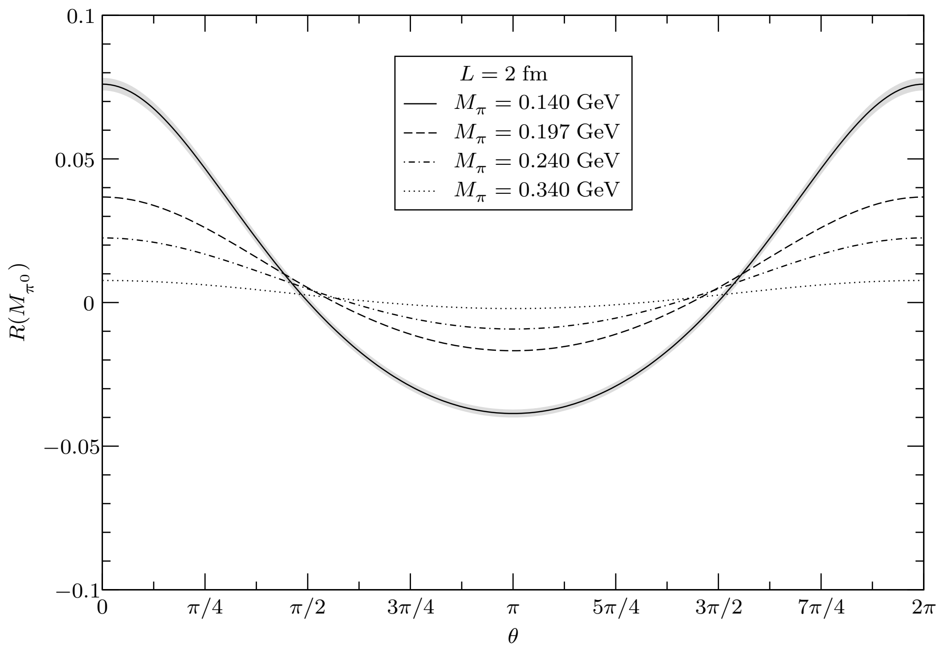
Masses

In Fig. 5.20—5.22 we represent the mass corrections estimated with $R(M_{\pi^0})$, $R(M_{\pi^\pm})$, $R(M_{K^\pm})$, $R(M_\eta)$. The pion mass dependences of $R(M_{\pi^0})$, $R(M_{\pi^\pm})$ are represented in logarithmic graphs (see Fig. 5.20a and Fig. 5.21a) whereas the pion mass dependences of $R(M_{K^\pm})$, $R(M_\eta)$ are represented in a linear graph (see Fig. 5.22a). In these graphs the bands of the uncertainity are displayed for solid lines (i.e. for $\theta = 0$). Bands of different colors refer to different values of L: gray ($L = 2$ fm), light green ($L = 3$ fm), orange ($L = 4$ fm). Uncertainity bands are here calculated with the usual formula of the error propagation. As unique source of error, we have taken the uncertainities on the LEC contained in the integrals $I^{(4)}(M_{\pi^0}, \pi^0), \ldots, I^{(4)}(M_\eta, \pi^\pm)$. We remind the reader that the LEC and their uncertainities are listed in Tab. 5.1.

The logarithmic graphs illustrate the exponential decay $\mathcal{O}(\mathrm{e}^{-M_\pi L})$ of the corrections. In Fig. 5.20a the lines are almost straight and can be distinguished for different angles. In



(a) Pion mass dependence of $R(M_{\pi^0})$.



(b) Angle dependence of $R(M_{\pi^0})$.

Figure 5.20: Mass corrections of the neutral pion beyond NLO.

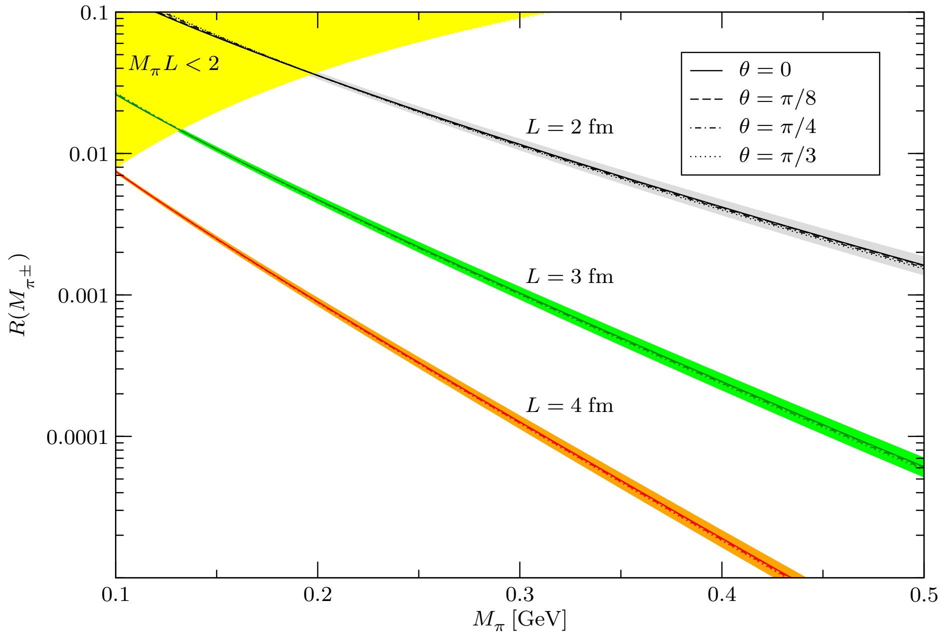
Table 5.3: Comparison of corrections evaluated at NLO with ChPT and estimated beyond NLO with asymptotic formulae. Here, we use $L = 2.83$ fm so that $M_\pi L = 2$ for $M_\pi = M_{\pi^\pm}^{\text{phys}}$. The uncertainities of $R(M_{\pi^0})$ originate from the errors of LEC contained in the integrals $I^{(4)}(M_{\pi^0}, \pi^0)$, $I^{(4)}(M_{\pi^0}, \pi^\pm)$. Note that results with $M_\pi < 0.140$ GeV should be taken with a grain of salt as they are in the region where the p-regime is no more guaranteed.

(a) Mass corrections for $\theta = 0$.

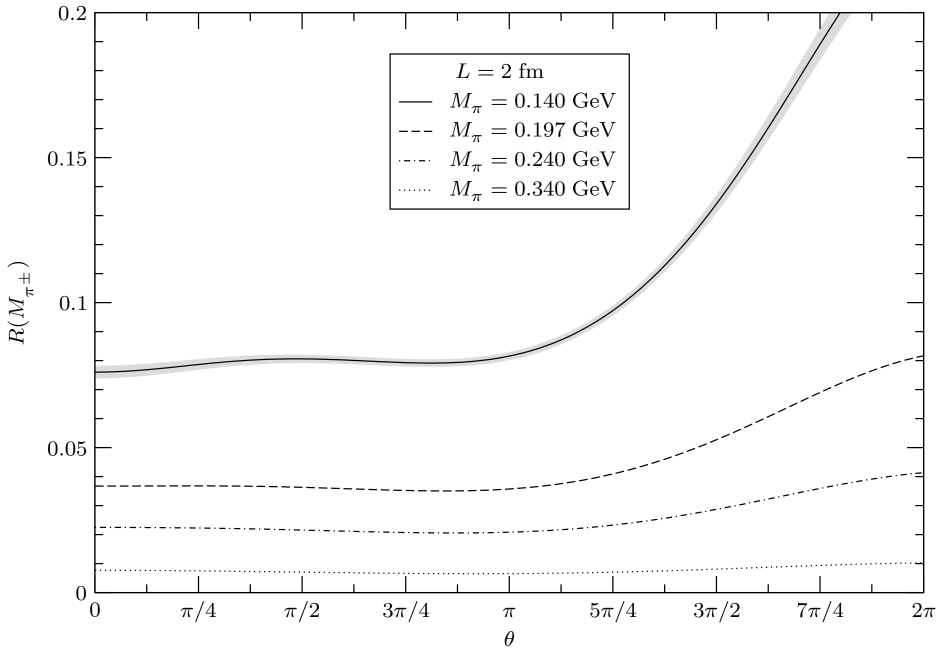
M_π [GeV]	δM_{π^0}	$R(M_{\pi^0})$
0.100	0.0240	0.0334(5)
0.120	0.0163	0.0234(5)
0.140	0.0113	0.0167(5)
0.160	0.0079	0.0121(4)
0.180	0.0057	0.0088(4)
0.200	0.0040	0.0065(3)
0.220	0.0029	0.0048(3)
0.240	0.0021	0.0038(2)
0.260	0.0015	0.0027(2)
0.280	0.0011	0.0020(2)
0.300	0.0008	0.0015(1)
0.320	0.0006	0.0012(1)
0.340	0.0004	0.0009(1)
0.360	0.0003	0.0007(1)
0.380	0.0002	0.0005(1)
0.400	0.0002	0.0004(0)
0.420	0.0001	0.0003(0)
0.440	0.0001	0.0002(0)
0.460	0.0001	0.0002(0)
0.480	0.0001	0.0001(0)
0.500	0.0000	0.0001(0)

(b) Mass corrections for $\theta = \pi/3$.

M_π [GeV]	δM_{π^0}	$R(M_{\pi^0})$
0.100	0.0050	0.0119(4)
0.120	0.0050	0.0102(4)
0.140	0.0043	0.0082(4)
0.160	0.0034	0.0065(4)
0.180	0.0027	0.0050(3)
0.200	0.0020	0.0039(3)
0.220	0.0015	0.0030(3)
0.240	0.0012	0.0023(2)
0.260	0.0009	0.0017(2)
0.280	0.0006	0.0013(2)
0.300	0.0005	0.0010(1)
0.320	0.0004	0.0008(1)
0.340	0.0003	0.0006(1)
0.360	0.0002	0.0005(1)
0.380	0.0001	0.0004(1)
0.400	0.0001	0.0003(0)
0.420	0.0001	0.0002(0)
0.440	0.0001	0.0002(0)
0.460	0.0000	0.0001(0)
0.480	0.0000	0.0001(0)
0.500	0.0000	0.0001(0)

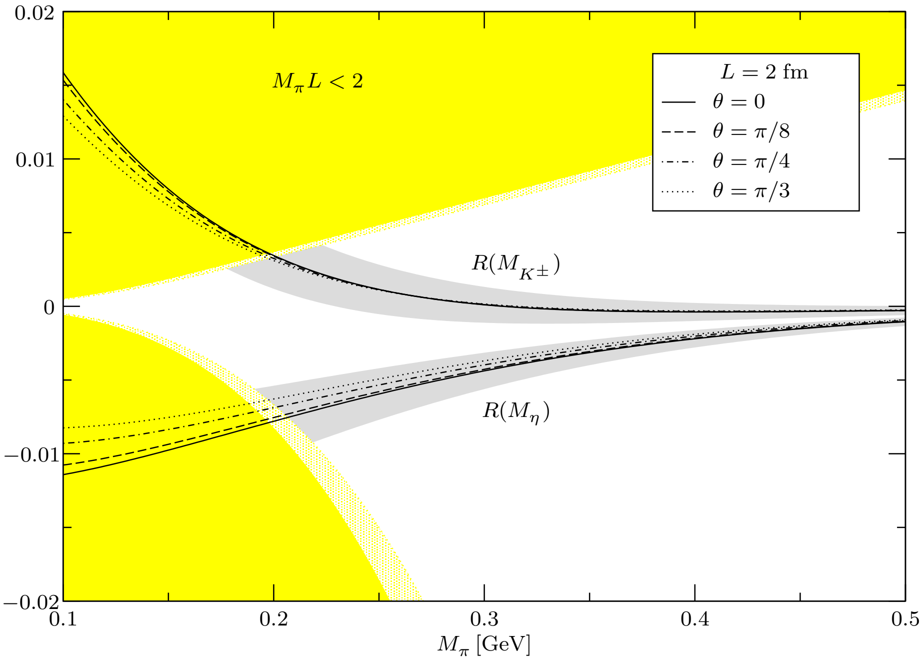


(a) Pion mass dependence of $R(M_{\pi^\pm})$.

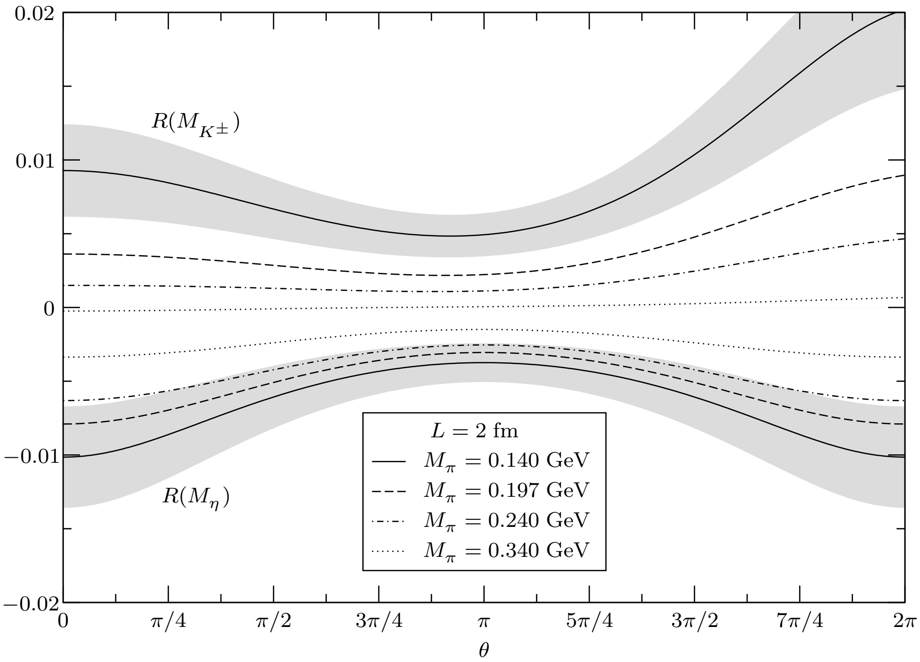


(b) Angle dependence of $R(M_{\pi^\pm})$.

Figure 5.21: Mass corrections of charged pions beyond NLO.



(a) Pion mass dependence of $R(M_{K^\pm})$, $R(M_\eta)$.



(b) Angle dependence of $R(M_{K^\pm})$, $R(M_\eta)$.

Figure 5.22: Mass corrections of charged kaons and eta meson beyond NLO.

Fig. 5.21a the lines are exactly straight and are so close that they overlap in the graph. If we consider $L = 2$ fm we read that $R(M_{\pi^0})$ is about 3.7% for $\theta = 0$ (resp. 1.9% for $\theta = \pi/3$) at $M_\pi \approx 0.2$ GeV and decreases to 0.2% for $\theta = 0$ (resp. 0.1% for $\theta = \pi/3$) at $M_\pi \approx 0.5$ GeV. Considering the same side length, $R(M_{\pi^\pm})$ is about 3.7% at $M_\pi \approx 0.2$ GeV and decreases to 0.2% at $M_\pi \approx 0.5$ GeV. These corrections are significantly bigger than those at NLO. For instance, in Tab. 5.3a (resp. Tab. 5.3b) we have listed numerical values for δM_{π^0}, $R(M_{\pi^0})$ at $L = 2.83$ fm for $\theta = 0$ (resp. for $\theta = \pi/3$). In some cases, $R(M_{\pi^0})$ is of order 50% with respect to δM_{π^0}. Such significant subleading effects were already observed in finite volume with PBC, see Ref. [24]. However, the comparison of numerical results with the asymptotic formula feeded by the amplitude at two loops [25,32] has showed that subsubleading effects are small and that the expansion does have a good converging behaviour for $M_\pi L > 2$. We are confident that this is also true for TBC and that subsubleading effects stay small, at least for small angles (i.e. $\theta < \pi$).

In Fig. 5.22a we represent the pion mass dependences of $R(M_{K^\pm})$, $R(M_\eta)$. The linear graph illustrates the exponential decay $\mathcal{O}(\mathrm{e}^{-M_\pi L})$ of the corrections. If we consider $L = 2$ fm, we read that $R(M_{K^\pm})$ is about 0.4% for $\theta = 0$ (resp. 0.3% for $\theta = \pi/3$) at $M_\pi \approx 0.2$ GeV and decreases to less than -0.1% at $M_\pi \approx 0.5$ GeV. Considering the same side length, $R(M_\eta)$ is about -0.8% for $\theta = 0$ (resp. -0.6% for $\theta = \pi/3$) at $M_\pi \approx 0.2$ GeV and amounts to -0.1% at $M_\pi \approx 0.5$ GeV. Here, subleading effects are almost of order 90%. The reason is that the contribution at NLO to $\delta M_{K^\pm}$ [resp. δM_η] is suppressed by $\mathcal{O}(\mathrm{e}^{-M_\eta L})$ [resp. $-M_\pi^2/M_\eta^2$] while the one beyond NLO is not. Note that $R(M_{K^\pm})$ may turn negative depending on M_π and is clearly not constant unlike Fig. 5.5a.

In Fig. 5.20b we represent the angle dependence of $R(M_{\pi^0})$. The gray band refers to the uncertainity for $M_\pi = 0.140$ GeV at $L = 2$ fm. We observe that $R(M_{\pi^0})$ depends on θ as a cosinus function. The corrections oscillate with a period of 2π and have maxima (resp. minima) at even (resp. odd) integer multiples of π. If we consider $M_\pi = 0.197$ GeV, the difference among maxima and minima is 5.4% at $L = 2$ fm. This difference is bigger than that at NLO and should be taken into account when physical observables are extrapolated from lattice data. Note that $R(M_{\pi^0})$ may turn negative for $\theta \in [3\pi/8, 13\pi/8]$ in a similar way as δM_{π^0} does at NLO.

In Fig. 5.21b we represent the angle dependence of $R(M_{\pi^\pm})$. We observe that $R(M_{\pi^\pm})$ depends on θ as $(a + \cos\theta)\sqrt{1+\theta^2}$ with $a > 0$. This dependence originates from contributions $\mathcal{O}(\xi_\pi^2)$ and provides large corrections at large angles. Here one should however retain only results in the interval $\theta \in [0, \pi]$. The reason is, $R(M_{\pi^\pm})$ was derived by means of the expansion (3.65) which is valid for small external twisting angles.

In Fig. 5.22b we represent the angle dependence of $R(M_{K^\pm})$, $R(M_\eta)$. We observe that $R(M_{K^\pm})$ depends on θ as $(a + \cos\theta)(b + \sqrt{1+\theta^2})$ with $b > a > 0$. This dependence originates from contributions $\mathcal{O}(\xi_\pi^2)$ and provides large corrections at large angles. However also in this case, one should retain only results for $\theta \in [0, \pi]$ as by derivation, $R(M_{K^\pm})$ is valid for small external twisting angles. In Fig. 5.22b the angle dependence of $R(M_\eta)$ corresponds to a negative cosinus. The maxima (resp. minima) are located at odd (resp. even) integer multiples of π. If we consider $M_\pi = 0.197$ GeV, the difference among maxima and minima is 0.5% at $L = 2$ fm. This difference is bigger than that at NLO but remains a negligible effect.

Renormalization Terms

In Fig. 5.23 and 5.24 we represent the renormalization terms estimated by means of $R^\mu(\vartheta_{\Sigma_{\pi^+}})$, $R^\mu(\vartheta_{\Sigma_{K^+}})$. We represent the first component as it is the only one which is non-zero for the configuration (5.7). The values on the y-axis are in given in GeV since $R^\mu(\vartheta_{\Sigma_{\pi^+}})$, $R^\mu(\vartheta_{\Sigma_{K^+}})$ are dimensionful quantities. Uncertainity bands are displayed for $\theta = \pi/8$ (see Fig. 5.23a and Fig. 5.24a) and for $M_\pi = 0.140$ GeV (see Fig. 5.23b and Fig. 5.24b).

In Fig. 5.23a [resp. Fig. 5.24a] we represent the pion mass dependence of $-R^\mu(\vartheta_{\Sigma_{\pi^+}})$ [resp. $-R^\mu(\vartheta_{\Sigma_{K^+}})$]. The logarithmic graphs illustrate the exponential decay $\mathcal{O}(\mathrm{e}^{-M_\pi L})$ of the renormalization terms. For $\theta \in \{\pi/8, \pi/4, \pi/3\}$ the absolute values of the renormalization terms increase with the angle. Note that the values are slightly bigger than those at NLO. Comparing Fig. 5.23a with Fig. 5.24a, we observe that for a fixed angle, $-R^\mu(\vartheta_{\Sigma_{\pi^+}})$ is bigger than $-R^\mu(\vartheta_{\Sigma_{K^+}})$.

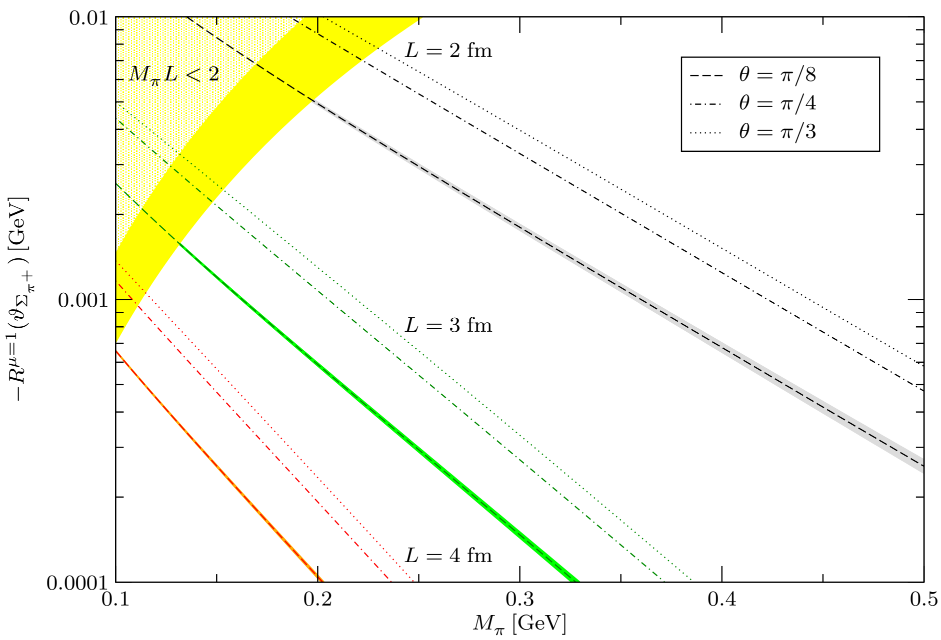
In Fig. 5.23b [resp. Fig. 5.24b] we represent the angle dependence of $R^\mu(\vartheta_{\Sigma_{\pi^+}})$ [resp. $R^\mu(\vartheta_{\Sigma_{K^+}})$]. We observe that the renormalization terms depend on θ nearly as negative sinus functions. The zeros correspond to integer multiples of π and the extrema (viz. minima and maxima) are close to half-integer multiples of π. Note that here, one should retain only results for $\theta \in [0, \pi]$ as by derivation, $R^\mu(\vartheta_{\Sigma_{\pi^+}})$, $R^\mu(\vartheta_{\Sigma_{K^+}})$ are valid for small external angles.

5.3.2 Decay Constants and Renormalization Terms of Axialvector Decay

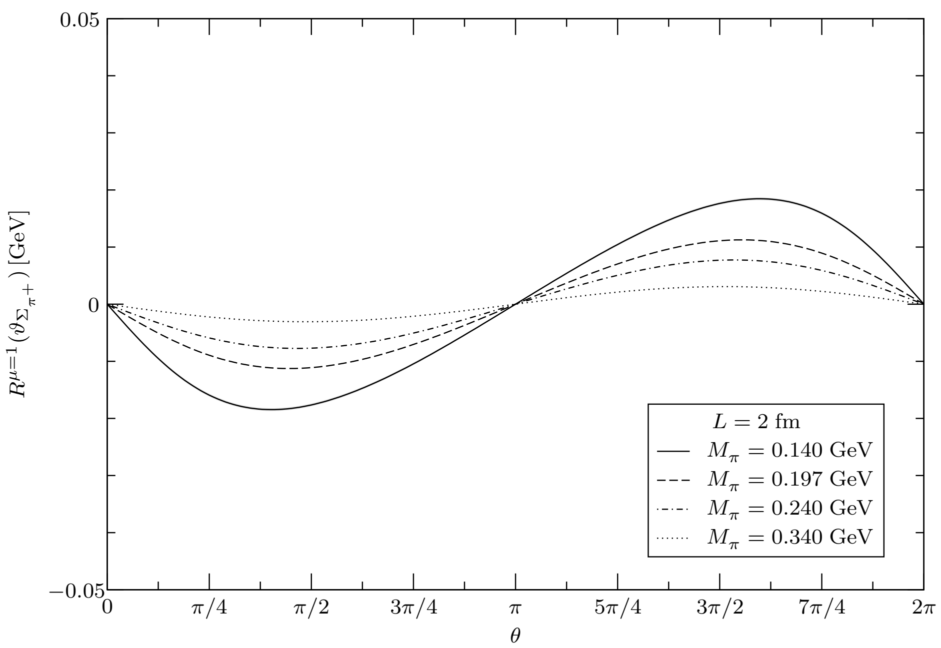
Decay Constants

In Fig. 5.25 and 5.26 we represent the corrections of decay constants estimated with $R(F_{\pi^\pm})$, $R(F_{K^\pm})$. The pion mass dependence of $-R(F_{\pi^\pm})$ [resp. $-R(F_{K^\pm})$] is represented in Fig. 5.25a [resp. Fig. 5.26a]. The logarithmic graphs illustrate the exponential decay $\mathcal{O}(\mathrm{e}^{-M_\pi L})$ of the corrections. The corrections are negative and for $\theta \in \{0, \pi/8, \pi/4, \pi/3\}$ their absolute values decrease with the angle. If we consider $L = 2$ fm, we read that $-R(F_{\pi^\pm})$ is about 11.3% for $\theta = 0$ (resp. 9.9% for $\theta = \pi/3$) at $M_\pi \approx 0.2$ GeV and decreases to 0.4% for $\theta = 0$ (resp. 0.3% for $\theta = \pi/3$) at $M_\pi \approx 0.5$ GeV. Considering the same side length, $-R(F_{K^\pm})$ is about 4.9% for $\theta = 0$ (resp. 3.9% for $\theta = \pi/3$) at $M_\pi \approx 0.2$ GeV and decreases to 0.1% at $M_\pi \approx 0.5$ GeV. These corrections are bigger than those of $R(M_{\pi^\pm})$, $R(M_{K^\pm})$. In general, they are also bigger than the corrections evaluated at NLO[2], as one can see e.g. from Tab. 5.4. Nonetheless, we observe that the value of $-R(F_{K^\pm})$ near to $M_\pi \approx 0.5$ GeV is slightly smaller than that of $-\delta F_{K^\pm}$ at the same pion mass. This can be explained as $R(F_{K^\pm})$ neglects the contributions of virtual kaons and eta

[2] In this case, subleading effects are under control (cfr. second and third columns of Tab. 5.4a and 5.4b)

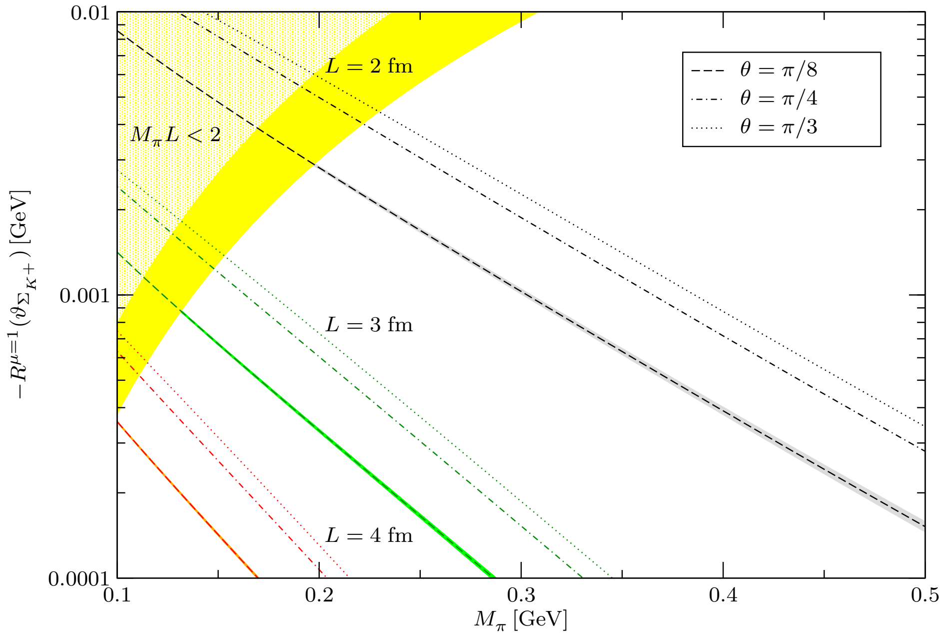


(a) *Pion mass dependence of* $-R^\mu(\vartheta_{\Sigma_{\pi^+}})$ *for* $\mu = 1$.

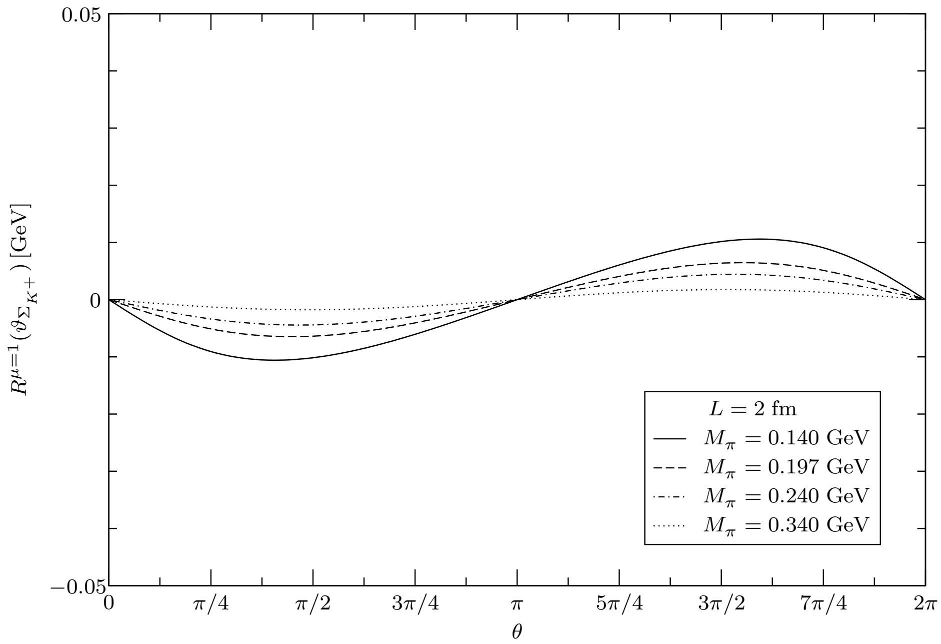


(b) *Angle dependence of* $R^\mu(\vartheta_{\Sigma_{\pi^+}})$ *for* $\mu = 1$.

Figure 5.23: Renormalization terms of charged pions beyond NLO. Note that in (a) the dark yellow area refers to the region $M_\pi L < 2$ *for* $\theta = \pi/8$.

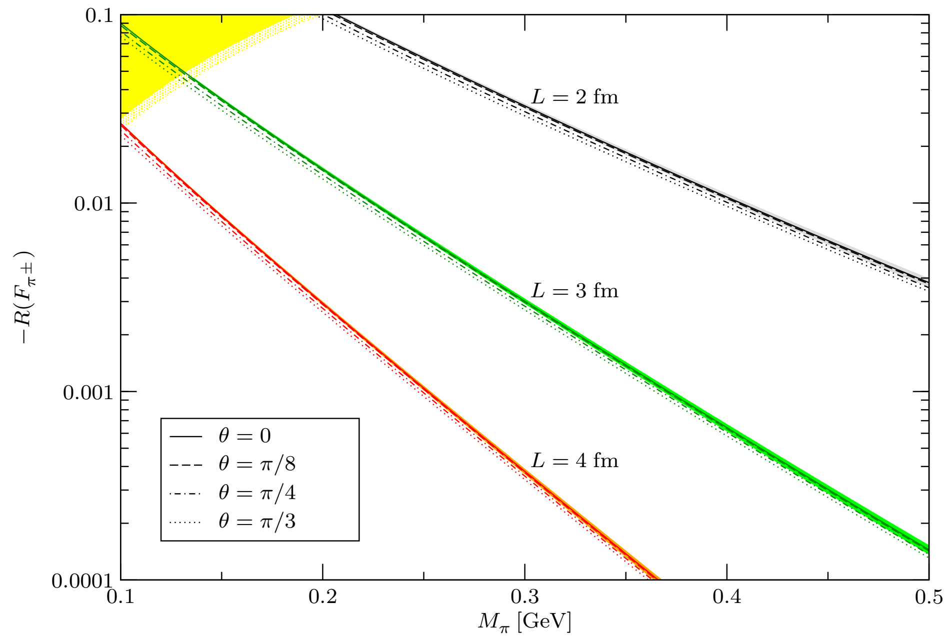


(a) Pion mass dependence of $-R^\mu(\vartheta_{\Sigma_{K^+}})$ for $\mu = 1$.

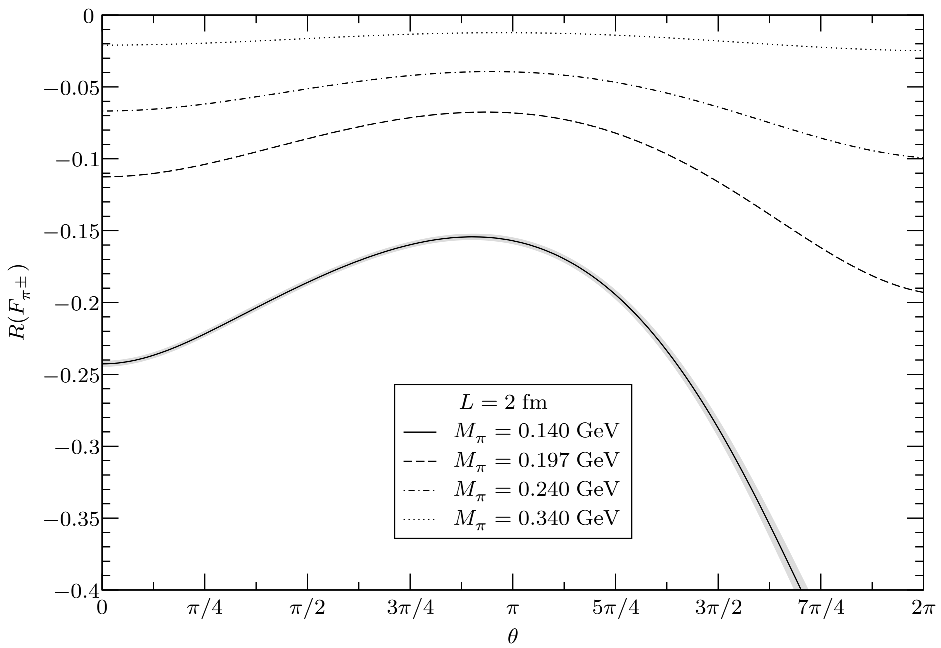


(b) Angle dependence of $R^\mu(\vartheta_{\Sigma_{K^+}})$ for $\mu = 1$.

Figure 5.24: Renormalization terms of charged kaons beyond NLO. Note that in (a) the dark yellow area refers to the region $M_\pi L < 2$ for $\theta = \pi/8$.



(a) Pion mass dependence of $-R(F_{\pi^\pm})$.



(b) Angle dependence of $R(F_{\pi^\pm})$.

Figure 5.25: Corrections of the decay constants of charged pions beyond NLO.

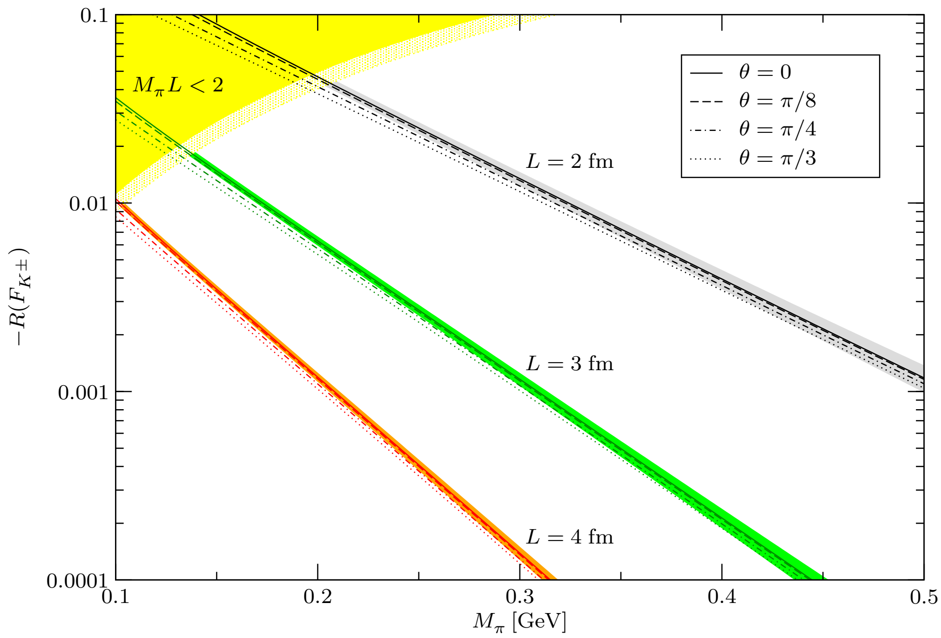
Table 5.4: Comparison of corrections evaluated at NLO with ChPT and estimated beyond NLO with asymptotic formulae. Here, we use $L = 2.83\,\mathrm{fm}$ so that $M_\pi L = 2$ for $M_\pi = M_{\pi^\pm}^{\mathrm{phys}}$. The uncertainities of $-R(F_{\pi^\pm})$ originate from the errors of LEC contained in the integrals $I^{(4)}(F_{\pi^\pm}, \pi^0), \ldots, I_D^{(4)}(F_{\pi^\pm}, \pi^\pm)$. Note that results with $M_\pi < 0.140\,\mathrm{GeV}$ should be taken with a grain of salt as they are in the region where the p-regime is no more guaranteed.

(a) Corrections for $\theta = 0$.

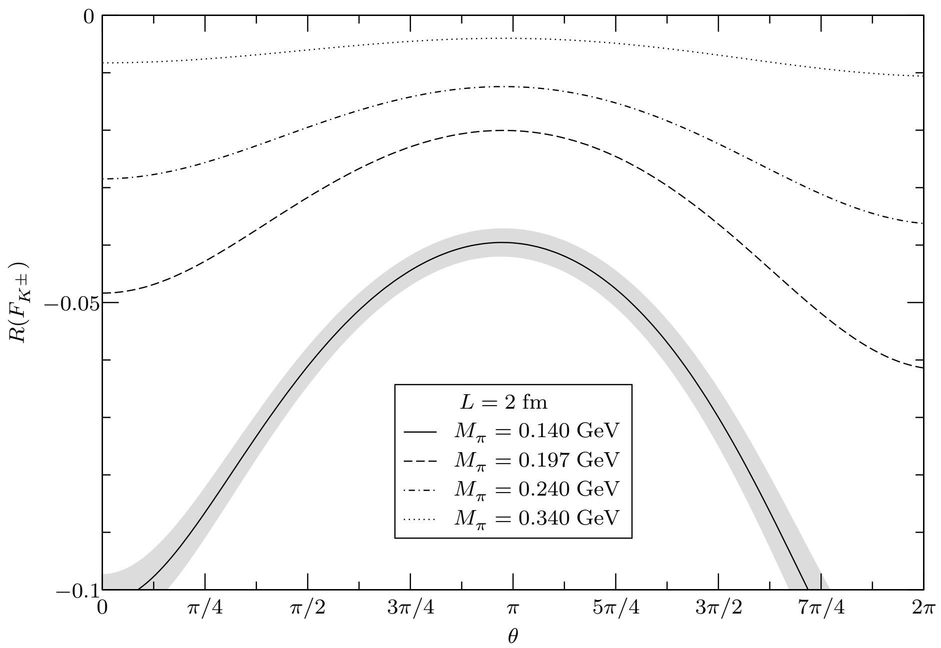
M_π [GeV]	$-\delta F_{\pi^\pm}$	$-R(F_{\pi^\pm})$
0.100	0.0961	0.1145(5)
0.120	0.0653	0.0789(4)
0.140	0.0454	0.0555(4)
0.160	0.0320	0.0395(3)
0.180	0.0228	0.0284(3)
0.200	0.0163	0.0206(2)
0.220	0.0118	0.0150(2)
0.240	0.0086	0.0110(2)
0.260	0.0062	0.0081(2)
0.280	0.0046	0.0060(1)
0.300	0.0034	0.0044(1)
0.320	0.0025	0.0033(1)
0.340	0.0018	0.0024(1)
0.360	0.0014	0.0018(1)
0.380	0.0010	0.0014(0)
0.400	0.0007	0.0010(0)
0.420	0.0006	0.0008(0)
0.440	0.0004	0.0006(0)
0.460	0.0003	0.0004(0)
0.480	0.0002	0.0003(0)
0.500	0.0002	0.0002(0)

(b) Corrections for $\theta = \pi/3$.

M_π [GeV]	$-\delta F_{\pi^\pm}$	$-R(F_{\pi^\pm})$
0.100	0.0772	0.0972(5)
0.120	0.0540	0.0679(4)
0.140	0.0383	0.0482(3)
0.160	0.0274	0.0346(3)
0.180	0.0200	0.0250(2)
0.200	0.0143	0.0182(2)
0.220	0.0104	0.0133(2)
0.240	0.0076	0.0098(2)
0.260	0.0056	0.0072(1)
0.280	0.0041	0.0053(1)
0.300	0.0030	0.0040(1)
0.320	0.0022	0.0029(1)
0.340	0.0016	0.0022(1)
0.360	0.0012	0.0016(1)
0.380	0.0009	0.0012(0)
0.400	0.0007	0.0009(0)
0.420	0.0005	0.0007(0)
0.440	0.0004	0.0005(0)
0.460	0.0003	0.0004(0)
0.480	0.0002	0.0003(0)
0.500	0.0002	0.0002(0)



(a) Pion mass dependence of $-R(F_{K^\pm})$.



(b) Angle dependence of $R(F_{K^\pm})$.

Figure 5.26: Corrections of the decay constants of charged kaons beyond NLO.

meson. In $\delta F_{K^\pm}$ these contributions are negligible but at $M_\pi \approx 0.5$ GeV they are of the same magnitude as that of virtual pions. In that case, the contribution of virtual pions is no more so dominant and $-R(F_{K^\pm})$ results slightly smaller than $-\delta F_{K^\pm}$.

In Fig. 5.25b [resp. Fig. 5.26b] we represent the angle dependence of $R(F_{\pi^\pm})$ [resp. $R(F_{K^\pm})$]. We observe that $R(F_{\pi^\pm})$, $R(F_{K^\pm})$ depend on θ nearly as $-(a+\cos\theta)(b+\sqrt{1+\theta^2})$ with variables $a, b > 0$. The variables are almost equal ($a \approx b$) for $R(F_{\pi^\pm})$ whereas $a > b$ for $R(F_{K^\pm})$. In both cases, the dependence provides large corrections at large angles. However, only results for $\theta \in [0, \pi]$ should be retained as by derivation, $R(F_{\pi^\pm})$, $R(F_{K^\pm})$ are valid for small external angles. We stress that $R(F_{\pi^\pm})$, $R(F_{K^\pm})$ can be comparable (or can be even larger) than the statistical precision of lattice simulations. In general, they should be taken into account by lattice practitioners when physical observables are extracted from lattice data.

Renormalization Terms

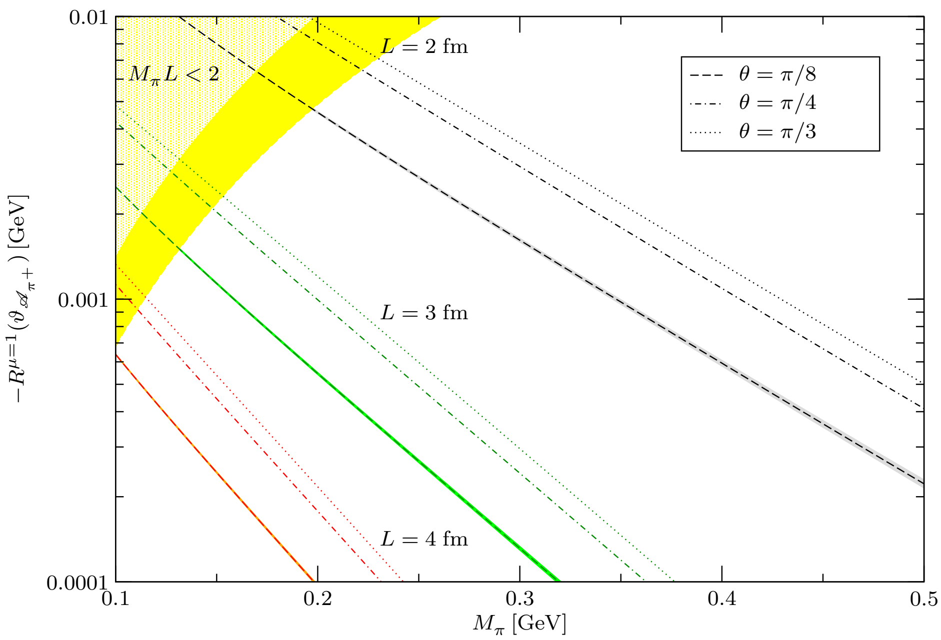
In Fig. 5.27 and 5.28 we represent the renormalization terms estimated with $R^\mu(\vartheta_{\mathscr{A}_{\pi^+}})$, $R^\mu(\vartheta_{\mathscr{A}_{K^+}})$. We represent the first component as it is the only one which is non-zero for the configuration (5.7). Since $R^\mu(\vartheta_{\mathscr{A}_{\pi^+}})$, $R^\mu(\vartheta_{\mathscr{A}_{K^+}})$ are dimensionful, the values on the y-axis are in given in GeV.

In Fig. 5.27a [resp. Fig. 5.28a] we represent the pion mass dependence of $-R^\mu(\vartheta_{\mathscr{A}_{\pi^+}})$ [resp. $-R^\mu(\vartheta_{\mathscr{A}_{K^+}})$]. The logarithmic graphs illustrate the exponential decay $\mathcal{O}(\mathrm{e}^{-M_\pi L})$ of the renormalization terms. Note that the absolute value of $R^\mu(\vartheta_{\mathscr{A}_{\pi^+}})$ is slightly bigger than that of $\Delta\vartheta^\mu_{\pi^+}$ at NLO. On the contrary, the absolute value of $R^\mu(\vartheta_{\mathscr{A}_{K^+}})$ is smaller than that of $\Delta\vartheta^\mu_{K^+}$. The reason is, $R^\mu(\vartheta_{\mathscr{A}_{K^+}})$ contains a factor F_π/F_K which reduces the absolute value, see Eq. (4.122). Comparing Fig. 5.27a with Fig. 5.23a we observe that for a fixed angle $-R^\mu(\vartheta_{\mathscr{A}_{\pi^+}})$ is smaller than $-R^\mu(\vartheta_{\Sigma_{\pi^+}})$. This difference is $\mathcal{O}(\xi_\pi^2)$ and is proportional to the renormalization terms $R^\mu(\vartheta_{\mathscr{G}_{\pi^+}})$ of Eq. (4.91). A similar observation can be made comparing Fig. 5.28a with Fig. 5.24a. For a fixed angle, $-R^\mu(\vartheta_{\mathscr{A}_{K^+}})$ is smaller than $-R^\mu(\vartheta_{\Sigma_{K^+}})$ where their difference is proportional to $R^\mu(\vartheta_{\mathscr{G}_{K^+}})$.

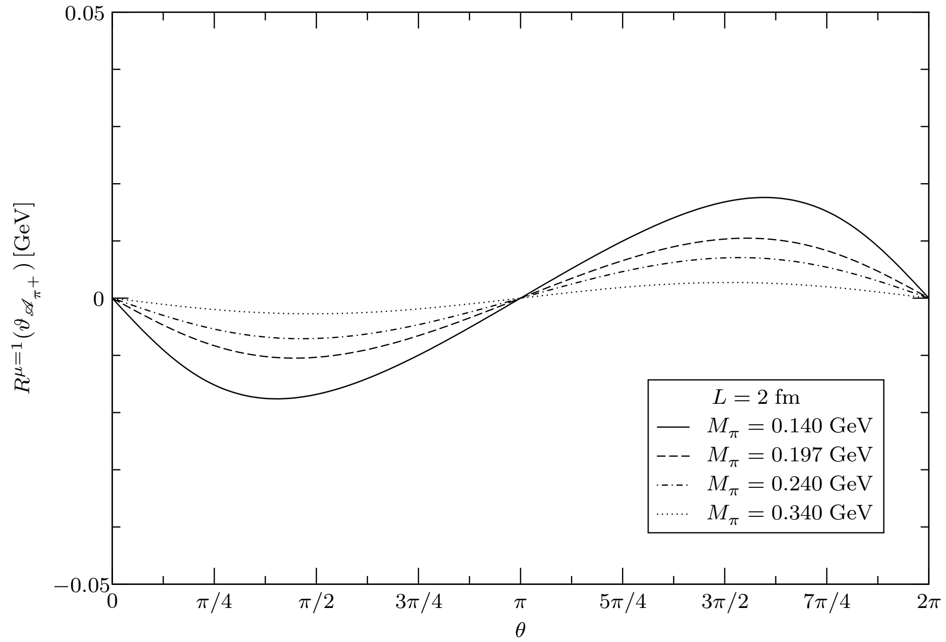
In Fig. 5.27b [resp. Fig. 5.28b] we represent the angle dependence of $R^\mu(\vartheta_{\mathscr{A}_{\pi^+}})$ [resp. $R^\mu(\vartheta_{\mathscr{A}_{K^+}})$]. We observe that $R^\mu(\vartheta_{\mathscr{A}_{\pi^+}})$, $R^\mu(\vartheta_{\mathscr{A}_{K^+}})$ depend on θ nearly as negative sinus functions. The zeros correspond to integer multiples of π and the extrema (viz. minima and maxima) are close to half-integer multiples of π. Note that only results for $\theta \in [0, \pi]$ should be retained as by derivation, $R^\mu(\vartheta_{\mathscr{A}_{\pi^+}})$, $R^\mu(\vartheta_{\mathscr{A}_{K^+}})$ are valid for small external angles.

5.3.3 Pseudoscalar Coupling Constants

In Fig. 5.29a we represent the pion mass dependence of $-R(G_{\pi^0})$. The logarithmic graphs illustrate the exponential decay $\mathcal{O}(\mathrm{e}^{-M_\pi L})$ of the corrections. In general, the corrections are negative and for $\theta \in \{\,0,\ \pi/8,\ \pi/4,\ \pi/3\,\}$ their absolute value increases with the angle. If we consider $L = 2$ fm, we read that $-R(G_{\pi^0})$ is about 3.9% for $\theta = 0$ (resp. 4.3% for $\theta = \pi/3$) at $M_\pi \approx 0.2$ GeV and decreases to about 0.1% at $M_\pi \approx 0.5$ GeV. In this case, the corrections are smaller than those at NLO. This can be explained if we look

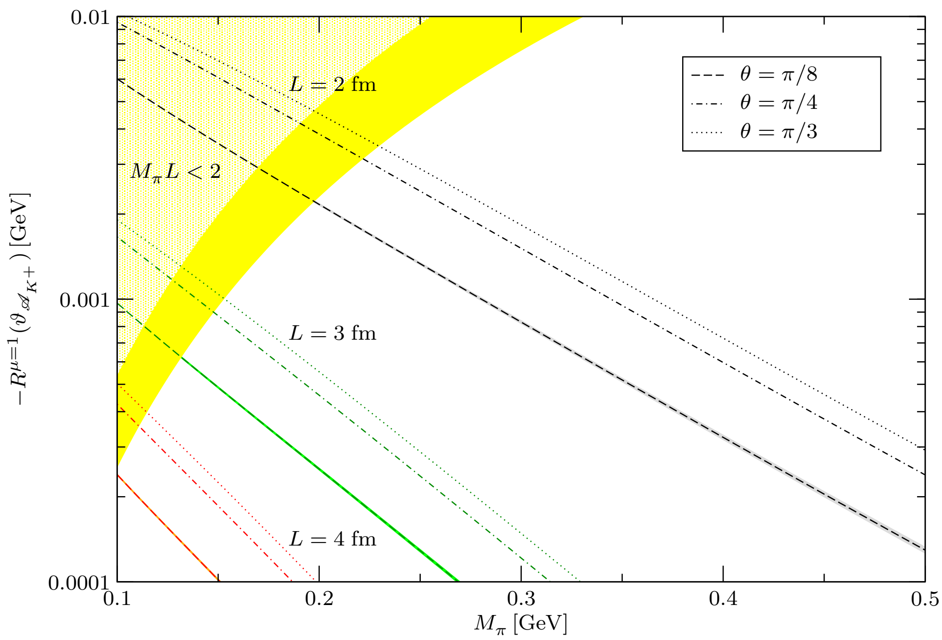


(a) Pion mass dependence of $-R^\mu(\vartheta_{\mathscr{A}_{\pi^+}})$ for $\mu = 1$.

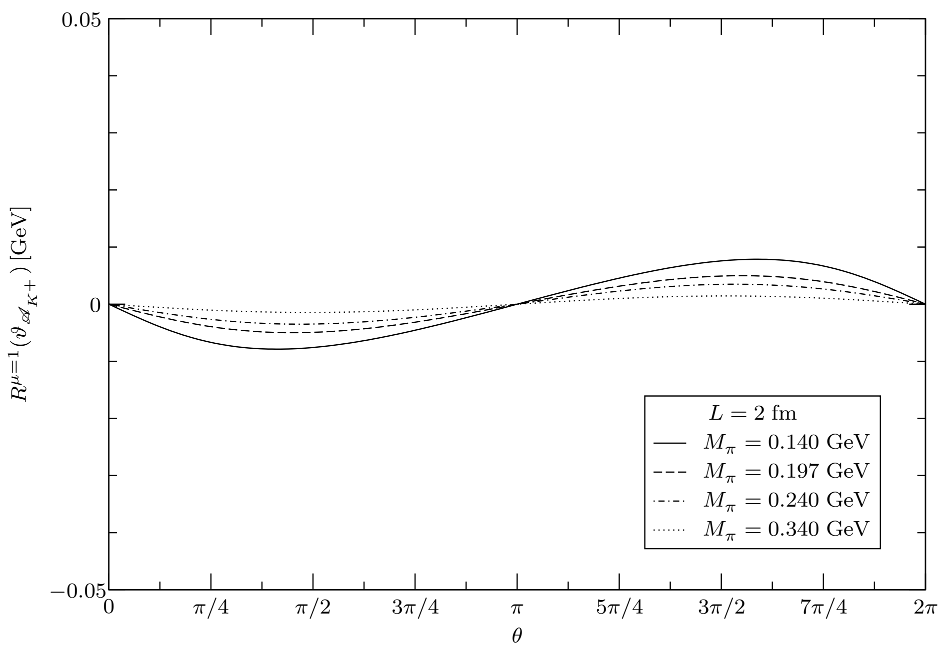


(b) Angle dependence of $R^\mu(\vartheta_{\mathscr{A}_{\pi^+}})$ for $\mu = 1$.

Figure 5.27: Renormalization terms of charged pions beyond NLO. Note that in (a) the dark yellow area refers to the region $M_\pi L < 2$ for $\theta = \pi/8$.



(a) Pion mass dependence of $-R^\mu(\vartheta_{\mathscr{A}_{K^+}})$ for $\mu = 1$.



(b) Angle dependence of $R^\mu(\vartheta_{\mathscr{A}_{K^+}})$ for $\mu = 1$.

Figure 5.28: Renormalization terms of charged kaons beyond NLO. Note that in (a) the dark yellow area refers to the region $M_\pi L < 2$ for $\theta = \pi/8$.

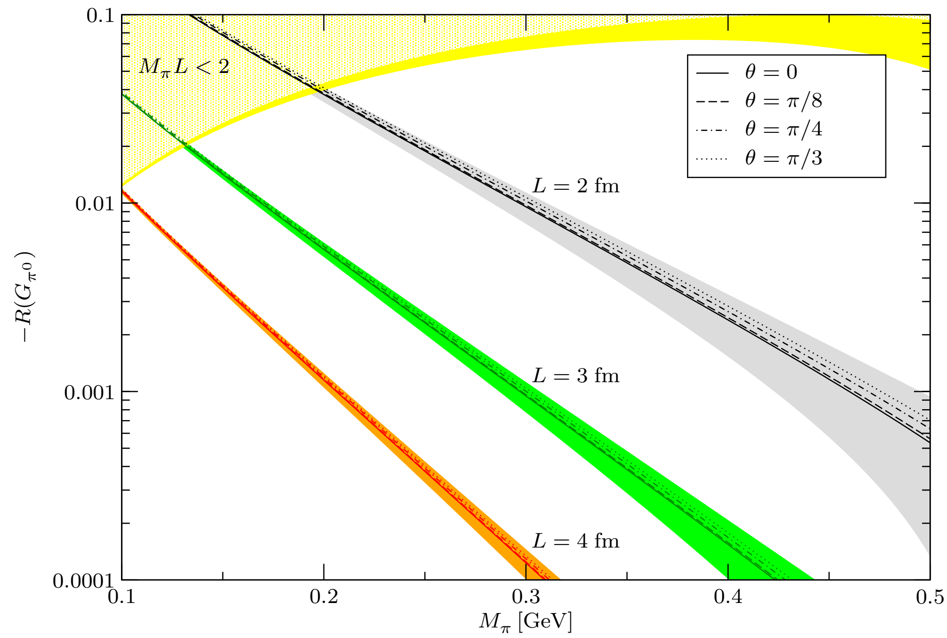
at the contributions $\mathcal{O}(\xi_\pi^2)$, see Eq. (4.82). For $\theta \in \{0, \pi/8, \pi/4, \pi/3\}$ the contribution originating from integral $I^{(4)}(G_{\pi^0}, \pi^0)$ is negative but that from $I^{(4)}(G_{\pi^0}, \pi^\pm)$ is positive. As the negative contribution is smaller than the positive one, the corrections estimated with $-R(G_{\pi^0})$ are smaller than those evaluated with $-\delta G_{\pi^0}$ at NLO.

In Fig. 5.29b we represent the angle dependence of $R(G_{\pi^0})$. We observe that $R(G_{\pi^0})$ depends on θ as a cosinus function. The function has minima (resp. maxima) located at even (resp. odd) integer multiples of π. Considering $L = 2$ fm, the difference among maxima and minima is 1.0% for $M_\pi = 0.197$ GeV. This difference is due to the contribution originating from $I^{(4)}(G_{\pi^0}, \pi^\pm)$.

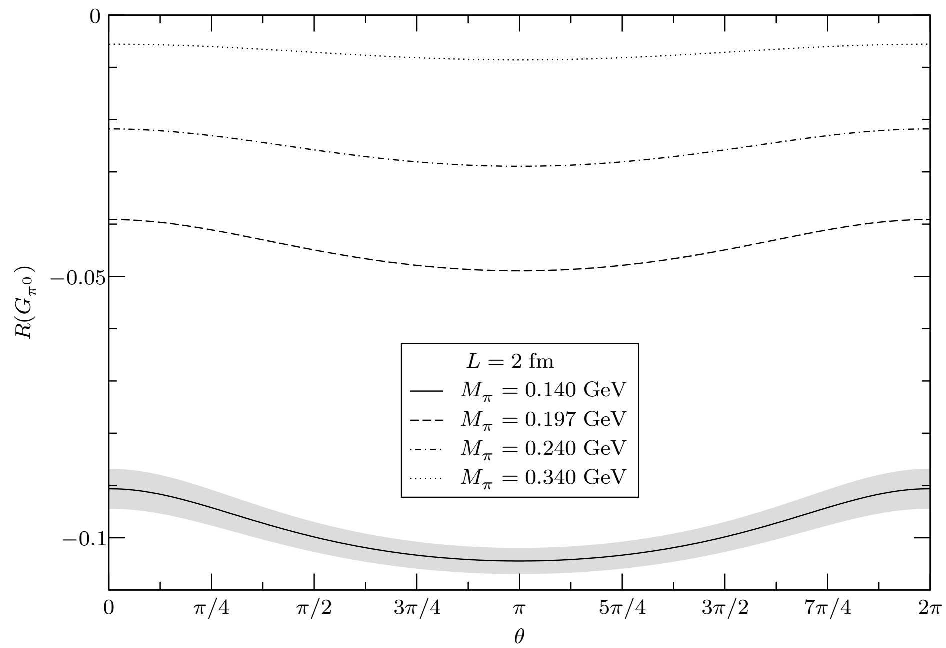
5.3.4 Pion Form Factors

We consider pions at rest and estimate the corrections of the matrix elements of the scalar form factor with $R(\Gamma_S^{\pi^0})$, $R(\Gamma_S^{\pi^+})$. In Fig. 5.30a [resp. Fig. 5.31a] we represent the pion mass dependence of $R(\Gamma_S^{\pi^0})$ [resp. $R(\Gamma_S^{\pi^+})$] at $q^2 = 0$. From the graphs we observe that the corrections decay exponentially as $\mathcal{O}(\mathrm{e}^{-M_\pi L})$. In general, they are negative but they may turn positive depending on the pion mass. If we consider $L = 2$ fm, we read that $R(\Gamma_S^{\pi^0})$ is about -0.4% for $\theta = 0$ (resp. 1.1% for $\theta = \pi/3$) at $M_\pi \approx 0.2$ GeV and amounts to -0.3% for $\theta = 0$ (resp. -0.2% for $\theta = \pi/3$) at $M_\pi \approx 0.5$ GeV. Considering the same side length, $R(\Gamma_S^{\pi^+})$ is about -0.4% for $\theta = 0$ (resp. 4.2% for $\theta = \pi/3$) at $M_\pi \approx 0.2$ GeV and amounts to -0.3% for $\theta = 0$ (resp. -0.2% for $\theta = \pi/3$) at $M_\pi \approx 0.5$ GeV. From these values, we see that $R(\Gamma_S^{\pi^0}) = R(\Gamma_S^{\pi^+})$ for $\theta = 0$ as expected in the case of PBC. However, note that at $M_\pi \approx 0.2$ GeV the corrections for $\theta = 0$ estimated with the asymptotic formulae are smaller –in absoulute value– than those evaluated at NLO: $-R(\Gamma_S^{\pi^0}) = -R(\Gamma_S^{\pi^+}) = 0.4\%$ whereas $-\delta\Gamma_S^{\pi^0} = -\delta\Gamma_S^{\pi^\pm} = 0.7\%$. This can be explained if we look at the contributions $\mathcal{O}(\xi_\pi^2)$, see Eqs. (4.98, 4.102). The contributions originating from $I^{(4)}(\Gamma_S^{\pi^0}, \pi^0), \ldots, I^{(4)}(\Gamma_S^{\pi^\pm}, \pi^\pm)$ are all positive for $\theta = 0$, $M_\pi \approx 0.2$ GeV and $L = 2$ fm. As the contributions originating from $I^{(2)}(\Gamma_S^{\pi^0}, \pi^0), \ldots, I^{(2)}(\Gamma_S^{\pi^\pm}, \pi^\pm)$ are all negative, the absolute value of $R(\Gamma_S^{\pi^0})$, $R(\Gamma_S^{\pi^+})$ is reduced and results smaller than that at NLO.

In Fig. 5.30b we represent the angle dependence of $R(\Gamma_S^{\pi^0})$ at $q^2 = 0$. We observe that $R(\Gamma_S^{\pi^0})$ depends on θ nearly as a negative cosinus function. The shape is slightly deformed due to the cancellation among $I^{(2)}(\Gamma_S^{\pi^0}, \pi^0)$, $I^{(2)}(\Gamma_S^{\pi^0}, \pi^\pm)$, see Eq. (4.98). In Fig. 5.31b we represent the angle dependence of $R(\Gamma_S^{\pi^+})$ at $q^2 = 0$. We observe that $R(\Gamma_S^{\pi^+})$ depends on θ nearly as $\theta \sin\theta$. This dependence originates from the last term of Eq. (4.100) and provides large corrections for large angles. In this case, only results for $\theta \in [0, \pi]$ should be retained as by derivation, $R(\Gamma_S^{\pi^+})$ is valid for small external angles.

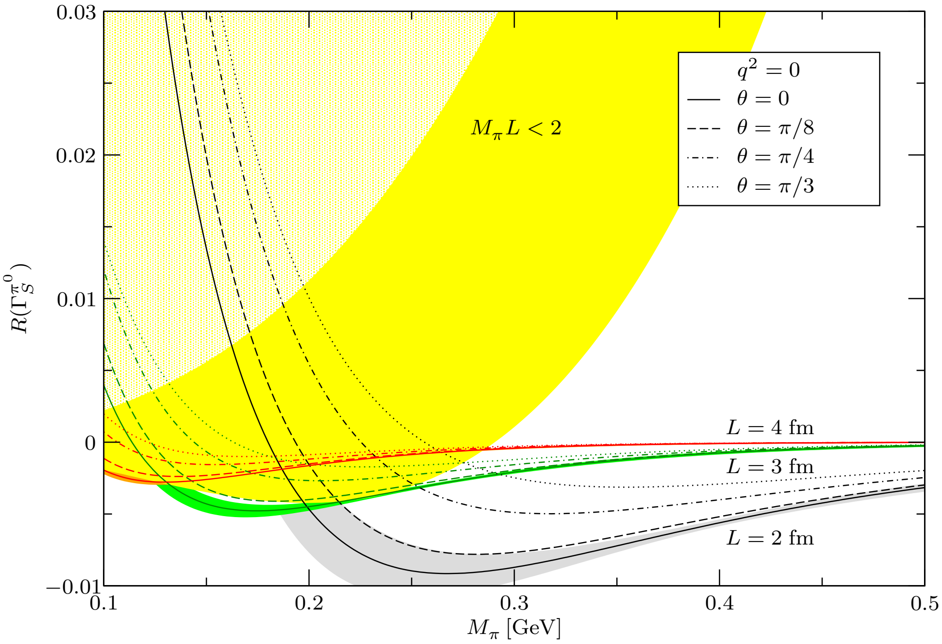


(a) Pion mass dependence of $-R(G_{\pi^0})$.

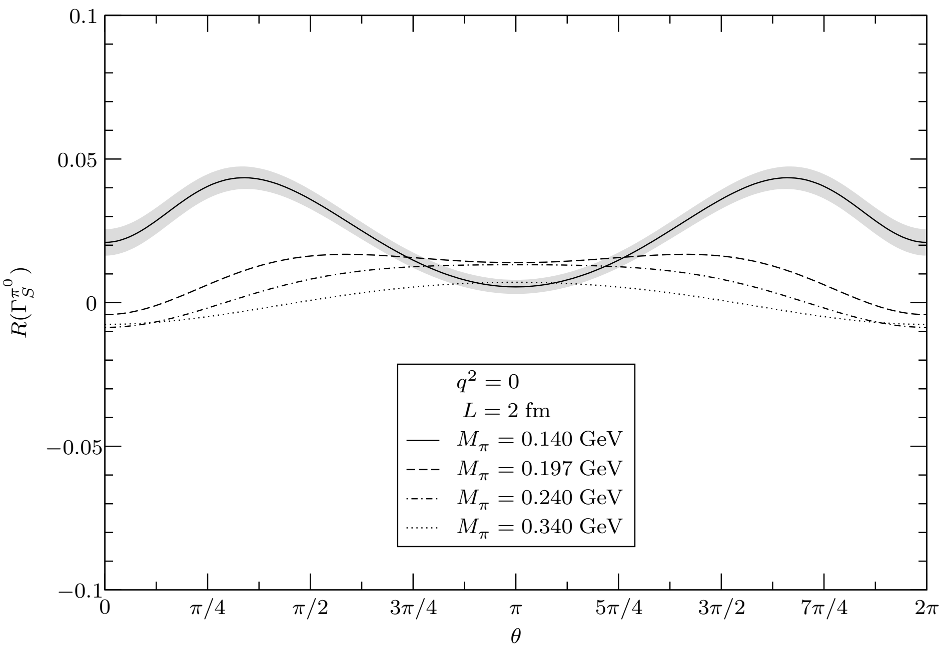


(b) Angle dependence of $R(G_{\pi^0})$.

Figure 5.29: Corrections of the pseudoscalar coupling constant of the neutral pion beyond NLO.

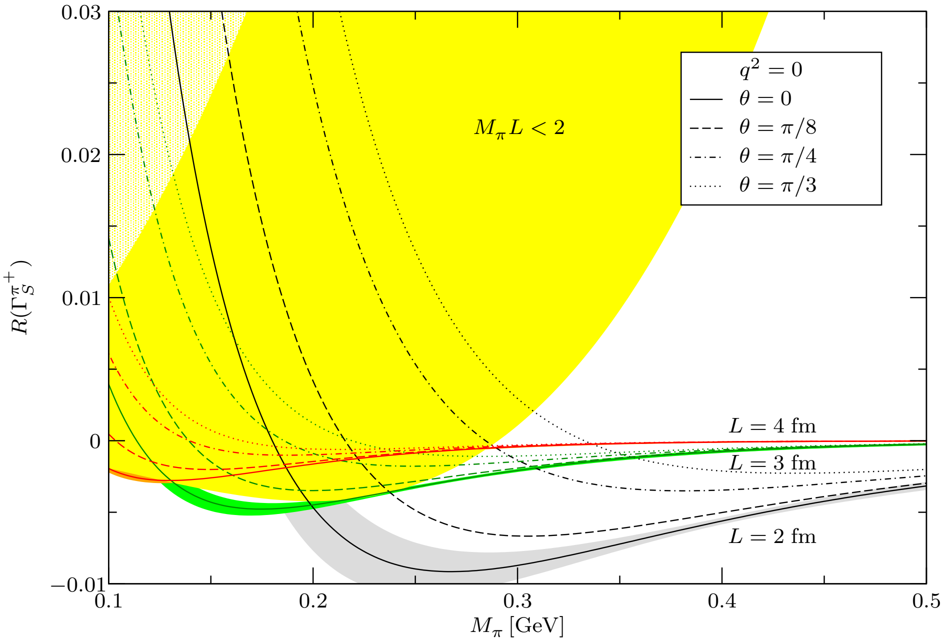


(a) Pion mass dependence of $R(\Gamma_S^{\pi^0})$ at $q^2 = 0$.

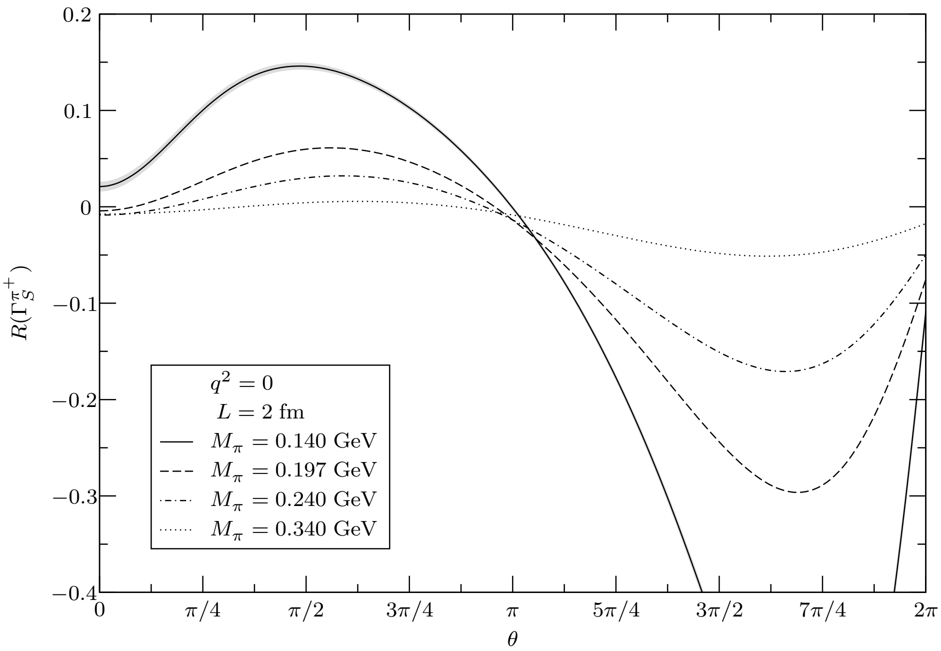


(b) Angle dependence of $R(\Gamma_S^{\pi^0})$ at at $q^2 = 0$.

Figure 5.30: Corrections of the matrix element of the scalar form factor beyond NLO.



(a) Pion mass dependence of $R(\Gamma_S^{\pi^+})$ at $q^2 = 0$.



(b) Angle dependence of $R(\Gamma_S^{\pi^+})$ at $q^2 = 0$.

Figure 5.31: Corrections of the matrix element of the scalar form factor beyond NLO.

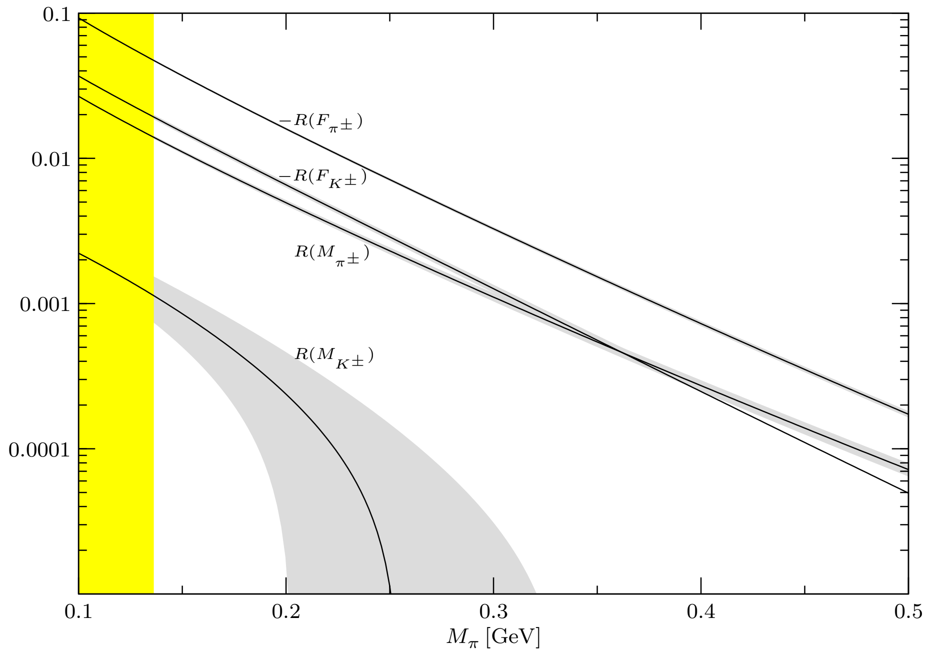


Figure 5.32: Corrections estimated beyond NLO with asymptotic formulae for the PACS-CS collaboration [49]. In gray are displayed the bands of the uncertainity. For $-R(F_{K^\pm})$ we have represented the uncertainity band only below $M_\pi \approx 0.360$ GeV as it overlaps the one of $R(M_{\pi^\pm})$. Above that value the uncertainities of $-R(F_{K^\pm})$ are similar to those of $R(M_{\pi^\pm})$. The yellow area refers to the region $M_\pi L < 2$ for $L = 2.90$ fm.

5.4 Numerical Applications

To conclude we illustrate two numerical applications of our formulae. We take lattice data from two collaborations: PACS-CS [49, 50] and ETM [51]. We adapt the numerical set-up and estimate the finite volume corrections for masses and decay constants. In both cases, we find corrections that are comparable (or even larger) than the statistical precision reached by the collaborations and hence, non-negligible.

5.4.1 Application to Data of PACS-CS

In Ref. [49] the PACS-CS collaboration simulates with $N_\mathrm{f} = 2 + 1$ dynamical flavors imposing PBC. They collect data at different values of the pion mass (from $M_\pi = 0.702$ GeV down to $M_\pi = 0.156$ GeV) and extrapolate physical observables to the physical point $M_\pi = M_{\pi^0}^{\mathrm{phys}}$. The PACS-CS data is presented in Tab. III, IV of [49] and the extrapolated results are summarized in Tab. X of [49] as well as Tab. II of [50]. We analyze these values and estimate the corrections at NLO and beyond that order.

For the analysis we adapt the numerical set-up as follows. Instead of Eq. (5.1) we use the expression of F_π at NLO obtained with 3-light-flavor ChPT, see Eq. (1.82). The parameters

F_0, $B_0 m_s$ are chosen as in Tab. VI (column "w/ FSE") of [49]. The values of LEC are taken from our Tab. 5.1 except those of $\bar{\ell}_3$, $\bar{\ell}_4$ and L_4^{r}, L_5^{r}, L_6^{r}, L_8^{r} which are taken from Tab. VI, IX (column "w/ FSE") of [49]. With this set-up, we have reproduced Fig. 18 of [49] representing the finite volume corrections evaluated by the PACS-CS collaboration at NLO. By means of asymptotic formulae, we estimate corrections beyond NLO as represented in Fig. 5.32.

The PACS-CS collaboration expects that at the side length $L = 2.90$ fm, the corrections of $-F_{\pi^\pm}(L)$, $-F_{K^\pm}(L)$, $M_{\pi^\pm}(L)$, $M_{K^\pm}(L)$ are less than 2% at the simulated point $M_\pi = 0.156$ GeV, see Ref. [49]. At NLO this is true for $-F_{K^\pm}(L)$, $M_{\pi^\pm}(L)$, $M_{K^\pm}(L)$ but not for $-F_{\pi^\pm}(L)$. We find that the corrections are about $-\delta F_{\pi^\pm} \approx 2.8\%$ at NLO and about $-R(F_{\pi^\pm}) \approx 3.3\%$ beyond NLO. These values are both bigger than 2%. However, if we look Tab. IV of [49] we see that the statistical precision reached by PACS-CS for the pion decay constant is about 5.3% and hence, larger than the corrections. In this case, the effects of finite volume corrections can be neglected.

At the physical point $M_\pi = M_{\pi^0}^{\mathrm{phys}}$ the PACS-CS collaboration expects corrections that are the same as at $M_\pi = 0.156$ GeV except those for the pion decay constant for which they expect values no more than 4% at NLO. This is true; but beyond NLO, we estimate corrections which are about $-R(F_{\pi^\pm}) \approx 4.8\%$ resp. $-R(F_{K^\pm}) \approx 2.0\%$ for the decay constants. If we look Tab. X (column "w/ FSE") of [49] we see that the statistical precision reached for the decay constants is less [3.4% in the case of $-F_{\pi^\pm}(L)$] or comparable [2.0% in the case of $-F_{K^\pm}(L)$] with the corrections we estimate. In this case, the effects of the corrections are non-negligible and should be taken into account.

5.4.2 Application to Data of ETM

In Ref. [51] the ETM collaboration simulates with $N_{\mathrm{f}} = 2 + 1 + 1$ dynamical flavors imposing PBC. The quark fields are Wilson twisted mass fermions at the maximal twist. In principle, one can apply twisted mass ChPT to evaluate the finite volume corrections as done in Ref. [26]. Here, we apply ChPT as done by the ETM collaboration but instead of the simplified formulae of Eq. (13) of [51] we use the full contributions given by the integrals (4.62, 4.74, D.2, D.6).

The ETM collaboration collects data for various runs at different values of L, M_π. The data is presented in Tab. 4, 8 of [51] and features an high statistical precision. From this data, are then extrapolated results for physical observables to the physical point $M_\pi = M_{\pi^0}^{\mathrm{phys}}$, see Tab. 9 of [51]. To perform the analysis, we adapt the numerical set-up of Section 5.1 as follows. The values of LEC are taken from our Tab. 5.1 except those of $\bar{\ell}_3$, $\bar{\ell}_4$ which are taken from Tab. 9 (column "combined") of [51]. The parameter F is determined evaluating Eq. (5.1) at $M_\pi = M_{\pi^0}^{\mathrm{phys}}$ in a similar way as in Section 5.1. In this case, we find

$$F = (85.6 \pm 0.2)\ \mathrm{MeV}, \qquad (5.13)$$

which is consistent with the result reported in Tab. 9 (column "combined") of [51]. The parameter $B_0 m_s$ is taken as in Section 5.1 and hence, values $B_0 m_s = 0.241\ \mathrm{GeV}^2$. If we

Table 5.5: Corrections evaluated at NLO with ChPT and estimated beyond NLO with asymptotic formulae for the ETM collaboration [51]. The runs are a part of those performed by the ETM collaboration, see Tab. 2, 3 of [51]. The statistical precision δ^{stat} is calculated using the data of Tab. 4, 8 [51]. Note that the runs A30.32 resp. B25.32 are those with the largest available volume for the ensembles A resp. B.

(a) Corrections of the pion decay constant.

Runs	M_π [GeV]	L [fm]	δ^{stat}	$-\delta F_{\pi^\pm}$	$-R(F_{\pi^\pm})$
A30.32	0.285	2.75	0.0054	0.0047	0.0062(1)
A40.24	0.333	2.06	0.0052	0.0127	0.0171(3)
A40.20	0.342	1.72	0.0105	0.0311	0.0415(6)
A60.24	0.397	2.06	0.0031	0.0059	0.0079(2)
B25.32	0.269	2.50	0.0063	0.0101	0.0134(2)
B85.24	0.489	1.88	0.0029	0.0039	0.0050(1)

(b) Mass corrections of pions.

Runs	M_π [GeV]	L [fm]	δ^{stat}	$\delta M_{\pi^\pm}$	$R(M_{\pi^\pm})$
A30.32	0.285	2.75	0.0029	0.0011	0.0021(1)
A40.24	0.333	2.06	0.0036	0.0029	0.0063(3)
A40.20	0.342	1.72	0.0062	0.0069	0.0155(8)
A60.24	0.397	2.06	0.0026	0.0013	0.0030(2)
B25.32	0.269	2.50	0.0037	0.0025	0.0046(2)
B85.24	0.489	1.88	0.0020	0.0008	0.0020(1)

(c) Mass corrections of kaons.

Runs	M_π [GeV]	L [fm]	δ^{stat}	$\delta M_{K^\pm}$	$R(M_{K^\pm})$
A30.32	0.285	2.75	0.0012	0.0000	$-0.0000(2)$
A40.24	0.333	2.06	0.0017	0.0001	$-0.0002(6)$
A40.20	0.342	1.72	0.0052	0.0005	$-0.0002(16)$
A60.24	0.397	2.06	0.0019	0.0001	$-0.0002(3)$
B25.32	0.269	2.50	0.0024	0.0000	0.0001(4)
B85.24	0.489	1.88	0.0018	0.0001	$-0.0003(3)$

insert this value in Eq. (5.3c) we find at $M_\pi = M_{\pi^0}^{\mathrm{phys}}$,

$$F_K = (0.107 \pm 0.004) \text{ GeV}, \tag{5.14}$$

which agrees with the result of PDG [2]. With this numerical set-up, we estimate the corrections reported in Tab. 5.5.

From Tab. 5.5a we observe that apart from the run A30.32 all corrections are larger than the statistical precision δ^{stat} of the ETM collaboration. The same can be said for most of the corrections[3] estimated with $R(M_{\pi^\pm})$, see Tab. 5.5b. On the contrary, we see from Tab. 5.5c that the mass corrections of kaons can be neglected for all the runs. For the largest avalaible volume of each ensemble (A and B) the ETM collaboration expects corrections that are within 1%; exceptions are the runs A60.24 and B85.24 for which they expect no more than 1.5%, see Ref. [51]. For the largest avalaible volumes (i.e. $L = 2.75$ fm for A resp. $L = 2.50$ fm for B) we confirm that the corrections are within 1% apart from the run B25.32 for which we estimate $-R(F_{\pi^\pm}) \approx 1.3\%$, see Tab. 5.5a. For the run A60.24 (resp. B85.24) we estimate corrections less than 0.2% (resp. 0.1%) at the largest avalaible volume. Nevertheless, the run B25.32 has corrections that –even though are conservatively estimated for $M_{\pi^\pm}(L)$ by ETM– are underestimated for $F_{\pi^\pm}(L)$. We stress that in this case, the corrections estimated with the asymptotic formulae [for both $M_{\pi^\pm}(L)$ and $F_{\pi^\pm}(L)$] are larger than the statistical precision δ^{stat}, see sixth row of Tab. 5.5a, 5.5b. Hence, for the run B25.32 the effects of corrections should be taken into account before physical observables could be extrapolated at the physical point.

[3] For mass corrections of pions we find subleading effects of order 50% (cfr. fifth and sixth columns of Tab. 5.5b). However, the analysis of Ref. [25,32] has showed that subsubleading effects are small and that the expansion does have a good converging behaviour for $M_\pi L > 2$.

Summary and Conclusions

In this work we have studied the effects of a finite cubic volume with twisted boundary conditions on pseudoscalar mesons. We have applied Chiral Perturbation Theory (ChPT) in the p-regime and introduced the twist by means of a constant vector field, see Ref. [36]. The corrections of masses, decay constants, pseudoscalar coupling constants, form factors were calculated at next-to-leading order (NLO) and estimated beyond that order through asymptotic formulae. A numerical analysis quantifies the importance of these corrections for generic situations and in the case of two real simulations [49–51].

In Chapter 2, we have calculated the corrections at NLO with ChPT and compared our expressions with Ref. [36–38]. In the calculations we have adopted the mass definition of Ref. [36, 37] which treats new extra terms as renormalization terms of the twisting angles. This is in contrast to other definitions such as e.g. that of Ref. [38]. The renormalization terms originate from the breaking of the cubic invariance introduced by the twist and are here reabsorbed in the on-shell conditions. This modifies the mass definition in finite volume. We have found that the corrections of masses as well as those of decay constants agree with Ref. [36]. We have detailed the derivations and presented results for the eta meson which agree with Ref. [38]. Relying on chiral Ward identities, we have calculated the corrections of pseudoscalar coupling constants. In these calculations, renormalization terms exactly cancel out because they are balanced on both sides of chiral Ward identities. At NLO the corrections of pseudoscalar coupling constants agree with Ref. [38]. This confirms that renormalization terms can be treated in different ways and that the definitions of Ref. [36, 37] and Ref. [38] are equivalent at NLO. However, we advocate to adopt the definition of Ref. [36,37] as it relies on mass poles with fixed locations just as considered in lattice simulation. This avoids further complications during the integration of correlator functions in momentum space. Successively, we have applied 2-light-flavor ChPT and calculated the corrections of the matrix elements of the pion form factors. We have presented results for the two cases: scalar and vector form factors. In the case of the vector form factor, the expressions agree with the results of Ref. [38]. Furthermore, we have showed that the Feynman–Hellman Theorem [39, 40] and the Ward–Takahashi identity [41–43] hold though the finite volume breaks Lorentz as well as cubic invariances. To prove the Ward–Takahashi identity we have constructed an effective field theory for charged pions which is invariant under electromagnetic gauge transformations and which reproduces the results obtained with ChPT at a vanishing momentum transfer. Such considerations were previously presented for periodic boundary conditions in Ref. [52] and are here generalized to twisted boundary conditions. Note that in finite volume, a necessary condition for the validity of the Ward–Takahashi identity is the discretization of the spatial components of the momentum transfer.

In Chapter 3, we have revised the derivation of Lüscher [23] and showed that it can be generalized to finite volume with twisted boundary conditions. We have derived asymptotic formulae for masses, decay constants, pseudoscalar coupling constants and scalar form factors. These formulae hold for arbitrary twisting angles in the case of the neutral pion and the eta meson. On the contrary, the formulae for charged pions and kaons were derived by means of an expansion which holds only if external twisting angles are small. Besides, we have derived asymptotic formulae for renormalization terms which are valid for small external twisting angles. Relying on chiral Ward identities, we have successively showed that the asymptotic formulae for masses, decay constants, pseudoscalar coupling constants are related to each other. A similar relation connects the asymptotic formulae for renormalization terms in an independent way. We have checked such relations for charged pions through a direct calculation. Then, starting from the Feynman–Hellman Theorem we have derived asymptotic formulae for pions, estimating the corrections of the matrix elements of the scalar form factor. These formulae are valid at a vanishing momentum transfer and in the case of charged pions, for small external twisting angles. We have also tried to derive more general formulae valid at a non-zero momentum transfer but we have not succeeded due to the complications introduced by the non-zero momentum transfer. Still, we have illustrated the steps undertaken and stressed that in principle, such complications should not arise if one considers matrix elements with two different external states, such as e.g. $\langle K^+| \, S_{4+i5} \, |\pi^0\rangle$.

In Chapter 4, we have applied the asymptotic formulae in combination with ChPT. We have worked out the amplitudes entering the formulae using the chiral representation at one loop taken from Ref. [10, 44–48]. The results were presented in terms of integrals as in Ref. [32] and allow one to estimate corrections beyond NLO in the chiral expansion. Cumbersome expressions were relegated in Appendix D.

In Chapter 5, we have estimated the corrections numerically. We have first performed a generic analysis adopting the numerical set-up of Ref. [25, 32]. In this case, the values of low-energy constants were taken –if available– from the FLAG working group [86]. Twisting angles were chosen in just one spatial direction and imposing twisted boundary conditions on just one flavor. This implies that we have performed the analysis with $|\vec{\vartheta}_{\pi^+}| = |\vec{\vartheta}_{K^+}| = \theta/L$ and $|\vec{\vartheta}_{K^0}| = 0$, where θ is a continuously varying angle. The corrections were estimated for volume of the side length $L = 2, 3, 4$ fm. For each of them, we have represented the dependences on the pion mass M_π and on the angle θ. In general, we have found that the corrections are modest and decay exponentially in $M_\pi L$. Still, for the smallest value of the p-regime (i.e. $M_\pi L \geq 2$) they can reach more than 10%. Such values can be comparable (or even larger) than the statistical precision of lattice simulations and should be then taken into account. Moreover, we have observed that for small twisting angles the corrections are similar to those with periodic boundary conditions. In the case $\theta \approx \pi$, the difference among corrections with periodic and twisted boundary conditions can reach a few percentage points. These are sizable effects. Thus, it is important to employ small angles in order to minimize these effects. At last, we have illustrated two possible numerical applications of our formulae. We have taken lattice data from the collaborations: PACS-CS [49, 50] and ETM [51]. In both cases, we have found corrections that were comparable (or even larger) than the statistical precision reached therein. Hence, we conclude that finite volume effects should be taken into account, especially in very precise lattice simulations.

The formulae presented in this work can be applied in two ways. One way is to choose the volume sufficiently large so that finite volume effects are minimized. Then, the corrections are negligible and the data of lattice simulations do not need to be corrected. The other way is to choose the volume small and correct the lattice data by means of our formulae. Choosing a small volume, one can save computational time which can be invested in some other way as e.g. to bring the limit of the lattice spacing (or of quark masses) closer to zero. In both cases, our formulae allow one to theoretically control the finite volume effects if external twisting angles are small.

Acknowledgements

On the journey that brought to the writing of this thesis I have met so many enlightened people who have showed me the way. It is impossible to mention all names but I feel that I am indebted to everyone at the Albert Einstein Center for Fundamental Physics at University of Bern.

I am infinitely grateful to Gilberto Colangelo for his incommensurable patience, his invaluable advices and innumerable encouragements. I hope that this work will partly repay him for the time he so kindly dedicated to me.

I am grateful to Christoph Häfeli for the many constructive discussions, the useful advices and for sharing with me his precious notes. These have fruitfully inspired parts of the present work and I hope that my words correctly captured his ideas.

I am also indebted to Stefan Lanz who has kindly supplied me with templates of his computer codes and notes. Both have been extremely useful in specific parts of this work.

I am thankful to Giovanni Villadoro, Johan Bijnens, Karim Ghorbani and Fu-Jiun Jiang for the private communications we had at different stages in this process and to Brian C. Tiburzi for accepting to co-referee this thesis.

A special mention goes to Markus Moser, Marco Steinacher, Matthias Nyfeler and Urs Gerber for "if everything [in the whole computer system] works as expected" is mainly thanks to them. I also would like to mention Urs Gerber for letting me use the LaTeX layout of his PhD thesis.

Infinite thanks go to the secretaries of the Institute for Theoretical Physics –Ottilia Hänni, Esther Fiechter and Ruth Bestgen– as without their help I would have been lost in an administrative jungle.

Moreover, I would like to thank my office colleagues who have supported me during all these years: Markus Moser, Matthias Nyfeler, Urs Gerber, Stefanie Marti, Massimiliano Procura, Andreas Crivellin, Michael Bögli, Vidushi Maillart and Stefano Maurizio. Thanks for the many conversations on Physics and especially, on unphysical topics.

In organizing my ideas, David Brémaud has helped me a lot: I thank him so much.

This work would hardly have been possible without the support, the generosity, and the love of Antonio and Elisabeth Vaghi–Ruch to whom I express my endless gratitude. I am also thankful to Katja Vaghi for the reciprocal support during the odyssey throughout our doctoral processes. Finally, to my two guiding stars that put me back on my path those times I was lost, Heike and Anton Bäßler, goes my fondest and deepest gratitude.

This work was partly funded by the Swiss National Foundation.

Appendix A

Sums in Finite Volume

We list some results that may be useful in the evaluation of loop diagrams in finite volume. For convenience, we define

$$\sumint' g(k) := \frac{1}{L^3} \sum_{\substack{\vec{k}=\frac{2\pi}{L}\vec{m} \\ \vec{m}\in\mathbb{Z}^3}} \int_{\mathbb{R}} \frac{\mathrm{d}k_0}{2\pi} g(k) - \int_{\mathbb{R}^4} \frac{\mathrm{d}^4 k}{(2\pi)^4} g(k), \tag{A.1}$$

where g is a generic function on momentum space and L is the side length of the finite cubic box. The right-hand side of the equation represents the difference among contributions in finite and infinite volume. For loop diagrams encountered in this work, this difference is finite and can be calculated by means of the Poisson resummation formula (2.6) and the direct integration. The first results we present, may be useful in the evaluation of tadpole diagrams. For $r \in \mathbb{N}$, we have

$$\sumint' \frac{\Gamma(r)}{i\left[M_P^2 - (k+\vartheta)^2\right]^r} = \frac{M_P^2}{(4\pi)^2}\, \mathrm{g}_r(\lambda_P, \vartheta) \tag{A.2a}$$

$$\sumint' \frac{\Gamma(r)\,(k+\vartheta)^\mu}{i\left[M_P^2 - (k+\vartheta)^2\right]^r} = -\frac{M_P^2}{(4\pi)^2}\, \mathrm{f}_r^\mu(\lambda_P, \vartheta) \tag{A.2b}$$

$$\sumint' \frac{\Gamma(r)\,(k+\vartheta)^\mu (k+\vartheta)^\nu}{i\left[M_P^2 - (k+\vartheta)^2\right]^r} = -\frac{M_P^2}{(4\pi)^2} \left[\frac{g^{\mu\nu}}{2}\, \mathrm{g}_{r-1}(\lambda_P, \vartheta) + \mathrm{h}_r^{\mu\nu}(\lambda_P, \vartheta)\right]. \tag{A.2c}$$

Here, $\Gamma(r)$ is the gamma function, $g^{\mu\nu}$ is the metric of Minkowski space-time, ϑ^μ is a twisting angle and $\lambda_P = M_P L$. The functions on the right-hand side can be expressed in terms of modified Bessel functions of the second kind, $K_r(x)$. They read

$$\mathrm{g}_r(\lambda_P,\vartheta) = \sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}} \frac{2}{M_P^2}\left[\frac{L^2|\vec{n}|}{2\lambda_P}\right]^{r-2} K_{r-2}(\lambda_P|\vec{n}|)\ \mathrm{e}^{iL\vec{n}\vec{\vartheta}} \tag{A.3a}$$

$$\mathrm{f}_r^\mu(\lambda_P,\vartheta) = \sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}} \frac{iL}{M_P^2}\, n^\mu \left[\frac{L^2|\vec{n}|}{2\lambda_P}\right]^{r-3} K_{r-3}(\lambda_P|\vec{n}|)\ \mathrm{e}^{iL\vec{n}\vec{\vartheta}} \tag{A.3b}$$

$$\mathrm{h}_r^{\mu\nu}(\lambda_P,\vartheta) = \sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}} \frac{L^2}{2M_P^2}\, n^\mu n^\nu \left[\frac{L^2|\vec{n}|}{2\lambda_P}\right]^{r-4} K_{r-4}(\lambda_P|\vec{n}|)\ \mathrm{e}^{iL\vec{n}\vec{\vartheta}}, \tag{A.3c}$$

where $n^\mu = \left(\begin{smallmatrix}0\\ \vec{n}\end{smallmatrix}\right)$. In Eqs. (2.30, 2.33) we have introduced the functions $\mathrm{g}_r(\lambda_P,\vartheta), \mathrm{f}_r^\mu(\lambda_P,\vartheta)$ for $r=1$.

To evaluate diagrams with different propagators one can use the Feynman parametrization,

$$\frac{1}{AB} = \int_0^1 \frac{\mathrm{d}z}{\big[zA+(1-z)B\big]^2}. \tag{A.4}$$

Here, we consider

$$A = M_P^2 - (k+\vartheta)^2 \tag{A.5a}$$
$$B = M_P^2 - (k+\vartheta+q)^2, \tag{A.5b}$$

where q^μ is a transfer momentum. The last results we present can be useful in the evaluation of fish diagrams. For $r\in\mathbb{N}$, we have

$$\not{\!\!\!\!\sum\!\!\!\!\!\int}{}'\ \frac{\Gamma(r)}{i\,[AB]^{\frac{r}{2}}} = \frac{M_P^2}{(4\pi)^2}\int_0^1 \mathrm{d}z\ \mathrm{g}_r(\lambda_z,q,\vartheta) \tag{A.6a}$$

$$\not{\!\!\!\!\sum\!\!\!\!\!\int}{}'\ \frac{\Gamma(r)\,(k+\vartheta)^\mu}{i\,[AB]^{\frac{r}{2}}} = -\frac{M_P^2}{(4\pi)^2}\int_0^1 \mathrm{d}z\ \left[\mathrm{f}_r^\mu(\lambda_z,q,\vartheta)+(1-z)q^\mu\,\mathrm{g}_r(\lambda_z,q,\vartheta)\right] \tag{A.6b}$$

$$\begin{aligned}\not{\!\!\!\!\sum\!\!\!\!\!\int}{}'\ \frac{\Gamma(r)\,(k+\vartheta)^\mu(k+\vartheta)^\nu}{i\,[AB]^{\frac{r}{2}}} &= \frac{M_P^2}{(4\pi)^2}\int_0^1 \mathrm{d}z\ \left\{(1-z)\left[\mathrm{f}_r^\mu(\lambda_z,q,\vartheta)q^\nu+\mathrm{f}_r^\nu(\lambda_z,q,\vartheta)q^\mu\right]\right\}\\ &\quad - \frac{M_P^2}{(4\pi)^2}\int_0^1 \mathrm{d}z\ \left[\frac{g^{\mu\nu}}{2}\,\mathrm{g}_{r-1}(\lambda_z,q,\vartheta)+\mathrm{h}_r^{\mu\nu}(\lambda_z,q,\vartheta)\right]\\ &\quad + \frac{M_P^2}{(4\pi)^2}\int_0^1 \mathrm{d}z\ \left[(1-z)^2 q^\mu q^\nu\,\mathrm{g}_r(\lambda_z,q,\vartheta)\right],\end{aligned} \tag{A.6c}$$

where $\lambda_z = M_P L\sqrt{1 + z(z-1)q^2/M_P^2}$. The functions on the RHS can be expressed as

$$\mathrm{g}_r(\lambda_z, q, \vartheta) = \sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}} \frac{2}{M_P^2}\left[\frac{L^2|\vec{n}|}{2\lambda_z}\right]^{r-2} K_{r-2}(\lambda_z|\vec{n}|)\ \mathrm{e}^{iL\vec{n}\left[\vec{\vartheta}+\vec{q}(1-z)\right]} \tag{A.7a}$$

$$\mathrm{f}_r^{\mu}(\lambda_z, q, \vartheta) = \sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}} \frac{iL}{M_P^2}\, n^{\mu}\left[\frac{L^2|\vec{n}|}{2\lambda_z}\right]^{r-3} K_{r-3}(\lambda_z|\vec{n}|)\ \mathrm{e}^{iL\vec{n}\left[\vec{\vartheta}+\vec{q}(1-z)\right]} \tag{A.7b}$$

$$\mathrm{h}_r^{\mu\nu}(\lambda_z, q, \vartheta) = \sum_{\substack{\vec{n}\in\mathbb{Z}^3\\|\vec{n}|\neq 0}} \frac{L^2}{2M_P^2}\, n^{\mu}n^{\nu}\left[\frac{L^2|\vec{n}|}{2\lambda_z}\right]^{r-4} K_{r-4}(\lambda_z|\vec{n}|)\ \mathrm{e}^{iL\vec{n}\left[\vec{\vartheta}+\vec{q}(1-z)\right]}. \tag{A.7c}$$

For $q^2 = 0$ the functions $\mathrm{g}_r(\lambda_z, q, \vartheta), \mathrm{f}_r^{\mu}(\lambda_z, q, \vartheta), \mathrm{h}_r^{\mu\nu}(\lambda_z, q, \vartheta)$ reduce to Eqs. (A.3a, A.3b, A.3c). In Eqs. (2.81, 2.84, 2.93b) we have introduced these functions for $r = 2$. Note that if $\vec{q} = \frac{2\pi}{L}\vec{l}$ with $\vec{l} \in \mathbb{Z}^3$, the results (A.6) can be simplify by means of substitutions $z \mapsto (1-z)$ and $\vec{n} \mapsto -\vec{n}$. This leads to the results of Sections 2.3.4 and Appendix B.2.

Appendix B

Gauge Symmetry in Finite Volume

To explain the results of Section 2.3.4 we construct an EFT for charged pions which is invariant under electromagnetic gauge transformations. The theory reproduces the expression obtained at a vanishing momentum transfer and indicates that the gauge symmetry is preserved in this case. Relying on this observation, we show that the Ward–Takahashi identity [41–43] holds in finite volume as long as the momentum transfer is discrete. Only the differential form of the identity –the Ward identity [114]– is violated due to the discretization of the spatial components. These considerations were presented for PBC in Ref. [52] and are here generalized to TBC.

B.1 Construction of an EFT Invariant under Gauge Symmetry

We consider a finite cubic box of the side length L on which we impose TBC. In presence of two light flavors, we can introduce the electromagnetic gauge field through the external vector field,

$$v^\mu = -eA^\mu(x)\,\mathcal{Q}. \tag{B.1}$$

Here, e is the elementary electric charge of the positron and $\mathcal{Q} = \mathrm{diag}(2/3, -1/3)$. As long as $\mathcal{Q}$ is diagonal we may redefine the fields so that they are periodic and introduce the twist as in Sections 2.3.4. The gauge field becomes periodic and satisfies

$$A^\mu(x + L\hat{e}_j) = A^\mu(x), \tag{B.2}$$

where $\hat{e}^\mu_j = \delta^\mu{}_j$ and $j = 1, 2, 3$. Since $A^\mu(x)$ is periodic we can expand the gauge field in Fourier modes

$$A^\mu(x) = \sum_{\substack{\vec{q}=\frac{2\pi}{L}\vec{l}\\ \vec{l}\in\mathbb{Z}^3}} \tilde{A}^\mu(x_0, \vec{q})\mathrm{e}^{i\vec{q}\vec{x}}. \tag{B.3}$$

We are interessed on the zero mode (i.e. $\vec{q} = \vec{0}$) from which we can study the electromagnetic form factor at a vanishing momentum transfer. To that end we separate the part of the gauge field containing the zero mode from the rest,

$$A^\mu(x) = A^\mu_{\mathrm{z}}(x_0) + A^\mu_{\mathrm{nz}}(x_0, \vec{x}). \tag{B.4}$$

Here,

$$A^\mu_{\mathrm{z}}(x_0) = \tilde{A}^\mu(x_0, \vec{0}\,) \tag{B.5a}$$

$$A^\mu_{\mathrm{nz}}(x_0, \vec{x}) = \sum_{\vec{q}\neq\vec{0}} \tilde{A}^\mu(x_0, \vec{q}\,)\mathrm{e}^{i\vec{q}\vec{x}}, \tag{B.5b}$$

where $A^\mu_{\mathrm{z}}(x_0)$ is the part containing the zero mode and $A^\mu_{\mathrm{nz}}(x_0, \vec{x})$ is the part containing non-zero modes. Note that the part containing the zero mode depends only on the time whereas the part containing non-zero modes is a periodic function in $\vec{x}$.

In general, the gauge field transforms under gauge transformations as

$$A^\mu(x) \mapsto A^\mu(x) + \partial^\mu\alpha(x). \tag{B.6}$$

Since $A^\mu(x)$ is periodic so must be $\partial^\mu\alpha(x)$. Thus, gauge transformations map periodic gauge fields into other periodic gauge fields. This assures that physical observables remain single valued in the finite cubic box.

We expand the gauge function in Fourier modes and separate the part containing the zero mode from the rest. We have

$$\alpha(x) = \alpha_{\mathrm{z}}(x_0, \vec{x}) + \alpha_{\mathrm{nz}}(x_0, \vec{x}), \tag{B.7}$$

where

$$\alpha_{\mathrm{z}}(x_0, \vec{x}) = \alpha_{\mathrm{z}}(x_0) + \vec{\alpha}\vec{x} \tag{B.8a}$$

$$\alpha_{\mathrm{nz}}(x_0, \vec{x}) = \sum_{\vec{q}\neq\vec{0}} \tilde{\alpha}(x_0, \vec{q}\,)\mathrm{e}^{i\vec{q}\vec{x}}. \tag{B.8b}$$

Here, $\vec{\alpha}$ is a constant vector and other irrelevant constants have been dropped. According to Eqs. (B.4, B.7) gauge transformations can be rewritten as

$$\begin{cases} A^\mu_{\mathrm{z}}(x_0) \mapsto A^\mu_{\mathrm{z}}(x_0) + \partial^\mu\alpha_{\mathrm{z}}(x_0, \vec{x}) \\ A^\mu_{\mathrm{nz}}(x_0, \vec{x}) \mapsto A^\mu_{\mathrm{nz}}(x_0, \vec{x}) + \partial^\mu\alpha_{\mathrm{nz}}(x_0, \vec{x}). \end{cases} \tag{B.9}$$

In particular, gauge transformations act on the part containing the zero mode as

$$A^\mu_{\mathrm{z}}(x_0) \mapsto A^\mu_{\mathrm{z}}(x_0) + \begin{cases} \partial^0\alpha_{\mathrm{z}}(x_0), & \mu = 0 \\ \vec{\alpha}, & \mu \neq 0. \end{cases} \tag{B.10}$$

As the part containing the zero mode depends only on the time the strength field tensor contains only the spatial components of $A^\mu_{\mathrm{z}}(x_0)$. Under gauge transformations the spatial components are translated by $\vec{\alpha}$ and this leaves the strength field tensor invariant. Hence, each spatial component of $A_{\mathrm{z}}^{\mu}(x_0)$ describes in the free theory a massless scalar particle.

We now couple matter fields. The gauge transformations act on quark fields as

$$q(x) \mapsto \mathrm{e}^{-ie\alpha(x)\mathcal{Q}} q(x). \tag{B.11}$$

Due to the field redefinition quark fields are periodic and satisfy $q(x + L\hat{e}_j) = q(x)$. In general, gauge transformations will not maintain the periodicity of quark fields. One can show that under gauge transformations the periodicity of quark fields is maintained if the constant vector takes the values

$$\vec{\alpha} = \frac{6\pi}{eL}\,\vec{m}, \qquad \text{with} \quad \vec{m} \in \mathbb{Z}^3. \tag{B.12}$$

This condition reduces the possible values of the gauge function and makes gauge transformations less general than in infinite volume. Thus, more operators –which are invariant under gauge transformations– can be built in the EFT.

We start the construction of the EFT considering two light quarks in presence of the electromagnetic interaction. At low energies the degrees of freedom of quarks are frozen and the relevant degrees of freedom are pions. We imagine that energies are so low that pions do not interact with themselves nor with other fields. All external fields can be integrated out. For simplicity, we just consider charged pions and set the field of the neutral pion to zero. In absence of the electromagnetic interaction the Lagrangian of the EFT reads

$$\mathcal{L} = \frac{1}{4}\left\langle \hat{D}_\mu \Phi [\hat{D}^\mu \Phi]^\dagger - M_{\pi^\pm}^2(L)\, \Phi^\dagger \Phi \right\rangle, \tag{B.13}$$

where

$$\Phi = \begin{pmatrix} 0 & \sqrt{2}\,\pi^+ \\ \sqrt{2}\,\pi^- & 0 \end{pmatrix}. \tag{B.14}$$

The mass $M_{\pi^\pm}(L)$ is the mass of charged pions in finite volume. The kinetic term contains the derivative

$$\hat{D}^\mu \Phi = \partial^\mu \Phi - i\left[w_\vartheta^\mu, \Phi\right], \tag{B.15}$$

where the twist is introduced by the constant vector field

$$w_\vartheta^\mu = \left(\vartheta_{\pi^+}^\mu + \Delta\vartheta_{\pi^+}^\mu\right)\frac{\tau_3}{2}. \tag{B.16}$$

The twisting angle $\vartheta_{\pi^+}^\mu$ and the renormalization term $\Delta\vartheta_{\pi^+}^\mu$ break Lorentz invariance. Such breaking is allowed as the theory is in finite volume with TBC. In the limit $\vartheta_{\pi^+}^\mu \to 0$ the constant vector field w_ϑ^μ disappears and the cubic invariance is restored: in this case the theory respects PBC. We note that $\Delta\vartheta_{\pi^+}^\mu$ resp. $M_{\pi^\pm}(L)$ may depend on parameters (like low-energy constants) that in the above theory are explicitly integrated out.

We add the electromagnetic interaction, including all possible operators which are invariant under gauge transformations. We limit ourselves to operators containing the zero mode. These are sufficient to study the electromagnetic form factor at a vanishing momentum transfer. By means of the minimal coupling prescription $\partial^\mu . \mapsto \partial^\mu . + ieA^\mu(x)[\mathcal{Q}, .]$ we make the kinetic term invariant under gauge transformations. Then, additional terms are allowed as Lorentz invariance is broken and as the constant vector $\vec{\alpha}$ is discrete, see Eq. (B.12). Such terms are responsible for the corrections of the electromagnetic form factor at a vanishing momentum transfer and for the screening of the electric charge in finite volume.

To construct the additional terms we use Wilson loops. We first consider the integral of the j-th spatial component of the gauge field,

$$\begin{aligned}\int_0^L \mathrm{d}x^j\, A^j(x) &= LA^j_{\mathrm{z}}(x_0) + \int_0^L \mathrm{d}x^j\, A^j_{\mathrm{nz}}(x_0, \vec{x}) \\ &= LA^j_{\mathrm{z}}(x_0) + L \sum_{\substack{\vec{q}\neq\vec{0} \\ q^j=0}} \tilde{A}^j(x_0, \vec{q})\mathrm{e}^{i\vec{q}\vec{x}}.\end{aligned} \tag{B.17}$$

Here, the repetition of j does not imply any sum and we have used the integral representation of Kronecker delta,

$$\frac{1}{L}\int_0^L \mathrm{d}x^j\, \mathrm{e}^{i\frac{2\pi}{L}\vec{l}\vec{x}} f(\vec{l}\,) = \delta_{l^j,0} f(\vec{l}\,), \qquad \vec{l} \in \mathbb{Z}^3. \tag{B.18}$$

The integral of the j-th spatial component of $A^j(x)$ gives the part of the gauge field containing modes with $q^j = 0$. Integrating over the three spatial components we isolate the zero mode,

$$\frac{1}{L^2}\int_{[0,L]^3} \mathrm{d}^3x\, A^j(x) = LA^j_{\mathrm{z}}(x_0). \tag{B.19}$$

By virtue of this result we form operators containing the zero mode and invariant under gauge transformations. For instance,

$$W^j = \exp\left[\frac{ie}{3L^2}\oint \mathrm{d}^3x\, A^j(x)\right], \tag{B.20}$$

where the integration is over a closed curve that cycles once in the finite cubic box. This operator represents a Wilson loop containing the zero mode of the gauge field. In principle, we may construct the remaining terms of the EFT by means of W^j. It is convenient to define Hermitian operators which transform in a manifest way under parity and charge conjugation. These operators are

$$W^j_+ = \frac{1}{2}\left[W^j + (W^j)^\dagger\right] \tag{B.21a}$$

$$W^j_- = \frac{1}{2i}\left[W^j - (W^j)^\dagger\right], \tag{B.21b}$$

and due to the unitarity of W^j, they are related as

$$W^j_+ = \left[1 - (W^j_-)^2\right]^{1/2}. \tag{B.22}$$

Hence, the remaining terms of the EFT can be constructed just with the operator W_-^j.

We can now write down the effective Lagrangian in presence of the electromagnetic interaction. Relying on the invariance on charge conjugation, parity, time reversal and gauge transformations, we obtain

$$\mathcal{L} = \frac{1}{4}\,\langle \hat{D}_\mu \Phi [\hat{D}^\mu \Phi]^\dagger - M_{\pi^\pm}^2(L)\,\Phi^\dagger \Phi\rangle - \frac{i}{2} Q(L)_{\mu\nu} W_-^\mu\,\langle \mathcal{Q}[(\hat{D}^\nu \Phi)^\dagger \Phi - \Phi^\dagger (\hat{D}^\nu \Phi)]\rangle + \ldots \tag{B.23}$$

Note that $W_-^\mu = \left(\begin{smallmatrix} 0 \\ \vec{W}_- \end{smallmatrix}\right)$ and

$$\hat{D}^\mu \Phi = \partial^\mu \Phi + ieA^\mu(x)[\mathcal{Q}, \Phi] - i\left[w_\vartheta^\mu, \Phi\right]. \tag{B.24}$$

The expression (B.23) needs some explanations. The dots at the end denotes that we have just written down the relevant terms of the effective Lagrangian. The most general effective Lagrangian contains terms with arbitrary many insertions of W_-^μ. Writing down all such terms is beyond our purpose. The expansion of W_-^μ starts with a term linear in $A_z^\mu(x_0)$ which is sufficient to study the electromagnetic form factor at a vanishing momentum transfer. The tensor $Q(L)^{\mu\nu}$ must be determined by matching. The tensor breaks the Lorentz as well as the cubic invariances and it is expected to disappear as $L \to \infty$. For $\vartheta_{\pi^+}^\mu = 0$ we expect that $Q(L)^{\mu\nu}$ reproduces the result for PBC, namely Eq. (33) of Ref. [52].

We match $Q(L)^{\mu\nu}$ with the results of Section 2.3.4. From the Lagrangian (B.23) we take the terms linear in $A_z^\mu(x_0)$ and evaluate them at the first order in e. We obtain

$$\langle \pi^\pm | J^\mu | \pi^\pm \rangle = 2e\,Q_e \left[(p + \vartheta_{\pi^\pm} + \Delta\vartheta_{\pi^\pm})^\mu + \frac{L}{3}\,(p + \vartheta_{\pi^\pm})_\nu Q(L)^{\mu\nu}\right] + \mathcal{O}(e^2), \tag{B.25}$$

where $Q_e = \pm 1$ is the electric charge of $\pi^\pm$ in elementary units. We match this expression with Eq. (2.96) and find

$$Q(L)^{\mu\nu} = \frac{6}{L}\,\xi_\pi\ \mathrm{h}_2^{\mu\nu}(\lambda_\pi, \vartheta_{\pi^+}). \tag{B.26}$$

The function $\mathrm{h}_2^{\mu\nu}(\lambda_\pi, \vartheta_{\pi^+})$ can be determined from Eq. (2.93b) and explicitly values

$$\mathrm{h}_2^{\mu\nu}(\lambda_\pi, \vartheta_{\pi^+}) = \sum_{\substack{\vec{n}\in\mathbb{Z}^3 \\ |\vec{n}|\neq 0}} 2\,\frac{n^\mu n^\nu}{|\vec{n}|^2}\ K_2(\lambda_\pi |\vec{n}|)\ \mathrm{e}^{iL\vec{n}\vec{\vartheta}} \qquad \text{with} \quad n^\mu = \begin{pmatrix} 0 \\ \vec{n} \end{pmatrix}. \tag{B.27}$$

As a check we control if the tensor (B.26) reproduces the result for PBC, i.e. Eq. (33) of Ref. [52]. We set $\vartheta_{\pi^\pm}^\mu = 0$ and contract the tensor with p_ν. Due to the cubic invariance we may write

$$\begin{aligned} p_\nu Q(L)^{\mu\nu} &= \frac{12}{L}\,\xi_\pi \sum_{\substack{\vec{n}\in\mathbb{Z}^3 \\ |\vec{n}|\neq 0}} p_\nu \frac{n^\mu n^\nu}{|\vec{n}|^2}\ K_2(\lambda_\pi |\vec{n}|) \\ &= \frac{4}{L}\,\xi_\pi\ p_\nu\left[g^{\mu\nu} - g^{\mu 0} g^{\nu 0}\right] \sum_{\substack{\vec{n}\in\mathbb{Z}^3 \\ |\vec{n}|\neq 0}} K_2(\lambda_\pi |\vec{n}|). \end{aligned} \tag{B.28}$$

The modified Bessel function can be expressed as

$$K_2(\lambda_\pi|\vec{n}|) = K_0(\lambda_\pi|\vec{n}|) + \frac{2}{\lambda_\pi|\vec{n}|}\, K_1(\lambda_\pi|\vec{n}|), \tag{B.29}$$

and we obtain

$$p_\nu Q(L)^{\mu\nu} = p_\nu \left[g^{\mu\nu} - g^{\mu 0} g^{\nu 0}\right] \underbrace{\frac{4\,\xi_\pi}{L}\left[K_0(\lambda_\pi|\vec{n}|) + \frac{2}{\lambda_\pi|\vec{n}|}\, K_1(\lambda_\pi|\vec{n}|)\right]}_{=\mathcal{Q}(L)}, \tag{B.30}$$

which coincides with Eq. (33) of Ref. [52].

The EFT described by (B.23) respects the gauge symmetry. It reproduces the result (2.96) at a vanishing momentum transfer. In the limit $\vartheta^\mu_{\pi^+} \to 0$ it reproduces the result for PBC of Ref. [52]. The presence of Wilson loops assures that the theory is invariant under gauge transformations. As long as $A^\mu(x)$ can be expanded in discrete Fourier modes this invariance is preserved. Hence, as long as the spatial components of the transfer momentum are discrete the results of Section 2.3.4 respect the gauge symmetry. In Appendix B.2 we show that in this case, the Ward–Takahashi identity holds in finite volume with TBC and that, the corrections of the vector form factor are related to the inverse propagator.

B.2 Ward–Takahashi Identity

In infinite volume the gauge symmetry imposes that the electromagnetic vertex function Γ^μ satisfies the Ward–Takahashi identity [41–43],

$$-iq_\mu \Gamma^\mu = iQ_e \left[\Delta^{-1}(p') - \Delta^{-1}(p)\right]. \tag{B.31}$$

Here, $q^\mu = (p' - p)^\mu$ is the momentum transfer, $\Delta(p')$ resp. $\Delta(p)$ are the propagators of outgoing and incoming particles and $Q_e = Q/e$ is the electric charge of external particles in elementary units. In the limit $q^\mu \to 0$, the identity tends to a differential form, known as Ward identity [114],

$$-i\Gamma^\mu = iQ_e \frac{\partial}{\partial p_\mu}\Delta^{-1}(p). \tag{B.32}$$

For external charged pions, we can calcultate the electromagnetic vertex function from the matrix elements

$$i\Gamma^\mu = \langle \pi^\pm(p')|\, V_3^\mu \,|\pi^\pm(p)\rangle\,. \tag{B.33}$$

In Ref. [10] these matrix elements are evaluated in ChPT at NLO and amount to

$$\Gamma^\mu = Q_e \left\{ (p' + p)^\mu \left[1 + f(q^2)\right] - \frac{q^\mu}{q^2}(p'^2 - p^2)\, f(q^2) \right\}, \tag{B.34a}$$

$$f(q^2) = \frac{1}{6F_\pi^2}\left[\left(q^2 - 4M_\pi^2\right)\bar{J}(q^2) + \frac{q^2}{(4\pi)^2}\left(\bar{\ell}_6 - \frac{1}{3}\right)\right] + \mathcal{O}(q^4). \tag{B.34b}$$

Here, we display all terms, even those that disappear as external momenta are on-shell. For on-shell momenta (i.e. $p^2 = p'^2 = M_\pi^2$) only the term proportional to $(p' + p)^\mu$ contributes and corresponds to the vector form factor (1.92).

The vertex function satisfies the Ward–Takahashi identity. This can be showed at NLO, contracting Eq. (B.34) with q_μ and arranging the survived terms in inverse propagators. The result can be formulated in the form of Eq. (B.31). In the limit $q^\mu \to 0$ the same vertex function satisfies the differential form of the identity, namely the Ward identity (B.32). These identities reflect that the electromagnetic current as well as the electric charge are conserved.

In finite volume the vertex function receives additional corrections,

$$\Gamma^\mu(L) = \Gamma^\mu + \Delta\Gamma^\mu. \tag{B.35}$$

Here, the first term corresponds to Eq. (B.34) with pion momenta shifted by $\vartheta^\mu_{\pi^\pm} = \pm\vartheta^\mu_3$ namely,

$$\Gamma^\mu = Q_e \left\{ P^\mu[1 + f(q^2)] - \frac{q^\mu}{q^2} (P_\nu q^\nu) f(q^2) \right\}, \tag{B.36}$$

where q^μ, P^μ are defined in Eqs. (2.79 2.82). The second term includes corrections arising from loop diagrams,

$$\begin{aligned}\Delta\Gamma^\mu = Q_e &\left\{ P^\mu \, \mathrm{G}_1 + 2\, \mathrm{H}_2^{\mu\nu} P_\nu - q^\mu \, \mathrm{F}_2^\nu P_\nu - \frac{P_\nu q^\nu}{q^2} \left[q^\mu \, \mathrm{G}_1 + 2\, \mathrm{H}_2^{\mu\rho} q_\rho - q^\mu \, \mathrm{F}_2^\rho q_\rho \right] \right\} \\ &+ Q_e \left\{ 2\Delta\vartheta^\mu_{\pi^\pm} + \left[2M_\pi^2 - (p' + \vartheta_{\pi^\pm})^2 - (p + \vartheta_{\pi^\pm})^2 - q^2 \right] \Delta\Theta^\mu_{\pi^\pm} \right\}. \end{aligned} \tag{B.37}$$

The Lorentz vectors $\Delta\vartheta^\mu_{\pi^\pm}, \Delta\Theta^\mu_{\pi^\pm}$ are defined in Eqs. (2.76, 2.83) and the new functions read

$$\mathrm{G}_1 = \xi_\pi \left[\int_0^1 \mathrm{d}z \; \mathrm{g}_1(\lambda_z, q, \vartheta_{\pi^+}) - \mathrm{g}_1(\lambda, \vartheta_{\pi^+}) \right] \tag{B.38a}$$

$$\mathrm{F}_2^\mu = \xi_\pi \int_0^1 \mathrm{d}z \; (1 - 2z)\, \mathrm{f}_2^\mu(\lambda_z, q, \vartheta_{\pi^+}) \tag{B.38b}$$

$$\mathrm{H}_2^{\mu\nu} = \xi_\pi \int_0^1 \mathrm{d}z \; \mathrm{h}_2^{\mu\nu}(\lambda_z, q, \vartheta_{\pi^+}). \tag{B.38c}$$

In the case of on-shell momenta, the second term $\Delta\Gamma^\mu$ reduces to the corrections (2.92). We note that

$$\begin{aligned} \mathrm{F}_2^\mu &= \frac{2}{q^2}\, q_\nu \, \mathrm{H}_2^{\mu\nu} \\ \Delta\Theta^\mu_{\pi^\pm} &= \pm\xi_\pi \int_0^1 \mathrm{d}z \; \left[\mathrm{f}_2^\mu(\lambda_z, q, \vartheta_{\pi^+}) + q^\mu \,(1/2 - z)\, \mathrm{g}_2(\lambda_z, q, \vartheta_{\pi^+}) \right] = \\ &= \pm\xi_\pi \int_0^1 \mathrm{d}z \; \left\{ \mathrm{f}_2^\mu(\lambda_z, q, \vartheta_{\pi^+}) - \frac{q^\mu}{q^2} \left[q_\nu \, \mathrm{f}_2^\nu(\lambda_z, q, \vartheta_{\pi^+}) \right] \right\}, \end{aligned} \tag{B.39}$$

if q^μ is non-vanishing momentum and if $\vec{q} = \frac{2\pi}{L}\vec{l}$ with $\vec{l} \in \mathbb{Z}^3 \setminus \{\vec{0}\}$. These relations can be showed by partial integration and by means of the properties of the derivatives of the modified Bessel functions of second kind.

We now show that here, the Ward–Takahashi identity holds in finite volume. We contract the vertex function (B.35) with q_μ and use the relations (B.39). The term $q_\mu \Delta\Theta^\mu_{\pi^\pm}$ disappears and many other cancel. The survived terms can be arranged to form inverse propagators,

$$\begin{aligned} -iq_\mu\Gamma^\mu(L) &= -iQ_e\left[q_\mu P^\mu + 2q_\mu\Delta\vartheta^\mu_{\pi^\pm}\right] = \\ &= iQ_e\left[\left(p+\vartheta_{\pi^\pm}\right)^2 + 2\left(p+\vartheta_{\pi^\pm}\right)_\mu \Delta\vartheta^\mu_{\pi^\pm} - \left(p'+\vartheta_{\pi^\pm}\right)^2 - 2\left(p'+\vartheta_{\pi^\pm}\right)_\mu \Delta\vartheta^\mu_{\pi^\pm}\right] \\ &= iQ_e\left[\Delta^{-1}_{\pi^\pm,L}(p') - \Delta^{-1}_{\pi^\pm,L}(p)\right]. \end{aligned} \tag{B.40}$$

In the last step of Eq. (B.40) we add terms canceling with each other in order to obtain the expression at NLO of propagators,

$$\Delta_{\pi^\pm,L}(p) = \frac{1}{M_\pi^2 - (p+\vartheta_{\pi^\pm})^2 - \Delta\Sigma_{\pi^\pm}}, \tag{B.41}$$

with $\Delta\Sigma_{\pi^\pm}$ given by Eq. (2.26b).

The demonstration of Eq. (B.40) shows that the Ward–Takahashi identity may hold in finite volume with TBC. Necessary conditions are: the discretization of q^μ and the renormalization due to $\Delta\vartheta^\mu_{\pi^\pm}$. The discretization of q^μ assures that the gauge symmetry is preserved and that the relations (B.39) are valid. The renormalization due to $\Delta\vartheta^\mu_{\pi^\pm}$ assures that the right-hand side of the identity can be arranged in inverse propagators. However, the continuous limit $q^\mu \to 0$ can not be taken due to the discretization of q^μ. This invalidates the differential form of the identity, i.e. the Ward identity (B.32). Note that the Ward identity is here violated in the spatial components but it remains valid in the zeroth component as q^0 is continuous.

Appendix C

Generalization (of the First Part) of the Derivation of Lüscher

To study the asymptotic behaviour of the self energy and derive Eqs. (3.28, 3.58) we must introduce some concepts of Abstract Graph Theory. We follow Ref. [23] and refer to [142] for further details.

C.1 Abstract Graph Theory

An (abstract) graph $\mathscr{G}$ consists of a finite set of lines $\mathscr{L}$, a non-empty finite set of vertices $\mathscr{V}$ and two maps $i, f\colon \mathscr{L} \to \mathscr{V}$. For every lines $\ell \in \mathscr{L}$ the image elements $i(\ell), f(\ell) \in \mathscr{V}$ represent the initial (resp. final) vertex of ℓ and are commonly called endpoints of ℓ. If the endpoints coincide, $i(\ell) = f(\ell)$, the line ℓ is a loop line.

In a graph $\mathscr{G}$ one can distinguish among different subsets of lines. Loops, paths, trees are all specific subsets of the line set $\mathscr{L}$. A loop in $\mathscr{G}$ is a non-empty subset $\mathscr{C} \subset \mathscr{L}$ with the property that there exists a sequence $v_1, v_2, \ldots, v_N$ of pairwise distinct vertices and a sequence $\ell_1, \ldots, \ell_N$ of lines in $\mathscr{C}$ such that v_k, v_{k+1} are endpoints of ℓ_k (for $k = 1, \ldots, N-1$) and v_N, v_1 are endpoints of ℓ_N. The simplest case is $\mathscr{C} = \{\, \ell \,\}$ where the loop $\mathscr{C}$ consists only of a loop line ℓ. In general, one can define an orientation for a loop $\mathscr{C}$ in $\mathscr{G}$. To every line $\ell \in \mathscr{C}$ one assigns a number $[\mathscr{C} : \ell] \in \{\, -1, 1 \,\}$ defined as

$$[\mathscr{C} : \ell] = \begin{cases} [\mathscr{C} : \ell'], & \text{if } i(\ell) = f(\ell') \\ -[\mathscr{C} : \ell'], & \text{if } i(\ell) = i(\ell') \text{ or } f(\ell) = f(\ell') \text{ for } \ell \neq \ell', \end{cases} \tag{C.1}$$

where i, f are the maps associated to $\mathscr{G}$.

Let $\mathscr{G}$ be a graph which connects two distinct vertices $a \neq b$ and let $\mathscr{L}$ be its line set. A subset $\mathscr{P} \subset \mathscr{L}$ is a path if there exists a sequence $a = v_1, v_2, \ldots, v_N = b$ of pairwise distinct vertices and a sequence $\ell_1, \ldots, \ell_{N-1}$ of lines in $\mathscr{P}$ such that v_k, v_{k+1} are endpoints of $\ell_k \in \mathscr{P}$ for all $k = 1, \ldots, N-1$. A path intersects another path if and only if they have a common line. The notion of paths enables us to introduce connected graphs. A graph $\mathscr{G}$ is connected if for any pair of distinct vertices $a \neq b$ there exists a path in $\mathscr{G}$ connecting

a, b. In a connected graph every vertex is an endpoint of some line except for the case where no lines exist and the graph is just a vertex.

Let $\mathscr{G}$ be a connected graph with the line set $\mathscr{L}$. A tree in $\mathscr{G}$ is a maximal subset $\mathscr{T} \subset \mathscr{L}$ not containing any loop in $\mathscr{G}$. If $\mathscr{T}$ is a tree and $a \neq b$ are two distinct vertices in $\mathscr{G}$ there exists an unique path $\mathscr{P} \subset \mathscr{T}$ connecting a, b. Furthermore, if we take the complement $\mathscr{T}^* = \mathscr{L} \setminus \mathscr{T}$, then for every lines $\ell^* \in \mathscr{T}^*$ there exists a unique loop in $\mathscr{G}$ which belongs to $\mathscr{T} \cup \{ \ell^* \}$. This loop neccessarily passes through the line ℓ^*.

One can remove lines from a graph $\mathscr{G}$. If one removes $\ell \in \mathscr{L}$ from $\mathscr{G}$ one obtains $\mathscr{G} \setminus \{ \ell \}$. The line set of the new graph is $\mathscr{L} \setminus \{ \ell \}$ but the set of vertices remains $\mathscr{V}$. Consequently, the maps of the new graph are $i, f \colon \mathscr{L} \setminus \{ \ell \} \to \mathscr{V}$. In an analogous way, one can remove a set of N lines. If $\mathscr{G}$ originally was a connected graph, the new graph $\mathscr{G} \setminus \{ \ell_1, \ldots, \ell_N \}$ generally decomposes in various connected components. A graph $\mathscr{G}$ is called N-particle irreducible between two vertices a, b, if the vertices a, b always belong to the same connectivity component of $\mathscr{G} \setminus \{ \ell_1, \ldots, \ell_N \}$ irrespective which of the lines $\ell_1, \ldots, \ell_N$ is removed.

The concepts introduced so far enable us to state a first result that we will need afterwards.

Lemma C.1.1. *In a connected graph $\mathscr{G}$ let $a \neq b$ be two distinct vertices and $\mathscr{C}_1, \ldots, \mathscr{C}_N$ pairwise disjoint loops. Then, there exists a path $\mathscr{P}$ in $\mathscr{G}$ connecting a, b such that either $\mathscr{P} \cap \mathscr{C}_j = \emptyset$ for all $j = 1, \ldots, N$ or $\mathscr{P} \cap \mathscr{C}_j$ is a path in $\mathscr{G}$ for all $j = 1, \ldots, N$.*

Proof. A proof of the Lemma can be found in Appendix A of Ref. [23]. □

On a graph $\mathscr{G}$ one can define gauge fields. As a gauge group one can choose $\mathbb{Z}^3$. A gauge field on $\mathscr{G}$ is an assignment of an integer vector $n^\mu(\ell) = \left[\begin{smallmatrix} 0 \\ \vec{n}(\ell) \end{smallmatrix} \right]$ to every line ℓ of the line set $\mathscr{L}$ of $\mathscr{G}$. A gauge field $n^\mu(\ell)$ is equivalent to another one, say $m^\mu(\ell)$, if they are related through the gauge transformation

$$m^\mu(\ell) = n^\mu(\ell) + \Delta\Lambda^\mu_\ell, \qquad \forall \ell \in \mathscr{L}. \tag{C.2}$$

Here, $\Delta\Lambda^\mu_\ell = \Lambda^\mu(f(\ell)) - \Lambda^\mu(i(\ell))$ where $\Lambda^\mu(v)$ is a field of integer vectors for each vertex $v \in \mathscr{V}$. The set of gauge fields equivalent to $n^\mu(\ell)$ forms an equivalence class which we denote by $[n]$. If $\mathscr{G}$ is a connected graph, $\mathscr{T}$ a tree in $\mathscr{G}$ and $[n]$ an equivalence class of gauge fields the representative field with

$$n^\mu(\ell) = 0, \qquad \forall \ell \in \mathscr{T}, \tag{C.3}$$

is called axial gauge field (relative to $\mathscr{T}$). One can show that in every class there exists a unique representative field which is an axial gauge field. Hence, the equivalence class can be characterized by the values of the axial gauge field along the complement $\mathscr{T}^* = \mathscr{L} \setminus \mathscr{T}$.

There are many kind of equivalence classes. Two important ones are the pure gauge configuration and the simple gauge configuration. The pure gauge configuration is the class of gauge fields equivalent to $n^\mu(\ell) = 0$, $\forall \ell \in \mathscr{L}$. The simple gauge configuration is the class of gauge fields equivalent to $n^\mu(\ell) = 0$, $\forall \ell \in \mathscr{L}$ except for one line ℓ^* which belongs to at least one loop in $\mathscr{G}$ and for which $|n(\ell^*)| = 1$. It is possible to construct a set of gauge independent simple fields in the following way. Consider $\mathscr{L}_c$ the set of lines $\ell \in \mathscr{L}$ belonging to at least one loop in $\mathscr{G}$. Two lines in $\mathscr{L}_c$ are independent if there exists a loop in $\mathscr{G}$ containing one of them but not the other. One chooses a maximal set of independent lines $\{ \ell_1, \ldots, \ell_N \} \subset \mathscr{L}_c$ and for $j = 1, \ldots, N$ one defines the simple fields,

$$n^\mu(\ell, j, \hat{e}) = \begin{cases} \hat{e}^\mu, & \text{if } \ell = \ell_j \\ 0, & \text{otherwise,} \end{cases} \tag{C.4}$$

where $\hat{e}^\mu = \left[\begin{smallmatrix} 0 \\ \hat{\vec{e}} \end{smallmatrix}\right]$, $\hat{\vec{e}} \in \mathbb{Z}^3$ with $|\hat{\vec{e}}| = 1$. Then, for $j = 1, \ldots, N$ the fields $n^\mu(\ell, j, \hat{e})$ form a complete list of gauge independent simple fields.

We conclude defining a quantity invariant under the gauge transformation (C.2). Let $\mathscr{C}$ be an oriented loop in $\mathscr{G}$ and $n^\mu(\ell)$ a gauge field on $\mathscr{G}$. Then,

$$W^\mu(\mathscr{C}, n) = \sum_{\ell \in \mathscr{C}} [\mathscr{C} : \ell] n^\mu(\ell) \tag{C.5}$$

is a gauge invariant quantity and corresponds to the Wilson loop of Lattice Gauge Theory.

C.2 Behaviour of the Self Energy at Large L

We consider a particle P in a finite cubic box of the side length L. At the boundaries we impose TBC and redefine the fields so that they are periodic. The nature of the particle P is not fundamental for the following discussion and for simplicity we assume that P is an hadron[1]. Our goal is to determine the behaviour of the self energy $\Delta\Sigma_P$ at large L.

We first study the behaviour of a generic contribution of the self energy. Note, however, that the results obtained in this section also hold (with appropriate modifications) for the derivative of the self energy. Let $\mathscr{D}$ be a Feynman diagram contributing to the self energy. To $\mathscr{D}$ we may assign an abstract graph $\mathscr{G}$ with the line set $\mathscr{L}$, the vertex set $\mathscr{V}$ and the maps $i, f \colon \mathscr{L} \to \mathscr{V}$. The graph $\mathscr{G}$ is one-particle irreducible and has two external vertices a, b, which may coincide. External vertices differ from common vertices as they are flowed by external momenta. In our case, the external momentum p^μ flows in a and goes out from b. Note that the momentum p^μ may be additionally shifted by the twisting angle ϑ_P^μ according to the flavor content of P.

In position space, the contribution $\mathscr{J}(\mathscr{D}, L)$ of the diagram $\mathscr{D}$ to the self energy takes the general form,

$$\mathscr{J}(\mathscr{D}, L) = \prod_{v \in \mathscr{V}'} \int_{\mathbb{R} \times [0,L]^3} \mathrm{d}^4 x(v) \; \mathbb{V} \left\{ \mathrm{e}^{-ip[x(b)-x(a)]} \prod_{\ell \in \mathscr{L}} G_\pi\left(\Delta x_\ell, L\right) \right\}. \tag{C.6}$$

Here, $\mathscr{V}' = \mathscr{V} \setminus \{ b \}$, $x^\mu(v)$ stands for the space-time coordinates of the vertex $v \in \mathscr{V}'$ and $\Delta x_\ell^\mu = x^\mu\left(f(\ell)\right) - x^\mu\left(i(\ell)\right)$ for $\ell \in \mathscr{L}$. The integrand is periodic and the integration

[1] This assumption does not change the argumentation of this section.

runs over $\mathbb{R} \times [0, L]^3$ where $\mathbb{R}$ represents the time axis and $[0, L]^3$ the finite cubic box. The integrand consists of products of operators and propagators. The quantity $\mathbb{V}$ is a product of vertex operators. These operators are differential operators originating from the Lagrangian. They correspond to vertex functions in momentum space. As the Lagrangian is independent from L [21] the vertex operators do not depend on L. However, they may depend on twisting angles of external and internal particles. The propagators are in finite volume. They are gathered in the product $\prod_{\ell \in \mathscr{L}} G_\pi(\Delta x_\ell, L)$. Each propagator is periodic and decays exponentially in L. Here, we retain only pion propagators as propagators of heavier particles decay more rapidly at large L.

To estimate the behaviour of $\mathscr{J}(\mathscr{D}, L)$ at large L we first work out the propagator $G_\pi(\Delta x_\ell, L)$. By virtue of the Poisson resummation formula (2.6) the propagator can be expressed as a sum over the gauge field $m^\mu(\ell)$,

$$G_\pi(\Delta x_\ell, L) = \sum_{m(\ell)} \int \frac{\mathrm{d}^4 k_\ell}{(2\pi)^4} \frac{\mathrm{e}^{ik_\ell[\Delta x_\ell + Lm(\ell)]}}{M_\pi^2 + (k_\ell + \vartheta_\ell)^2}, \tag{C.7}$$

where

$$\vartheta_\ell^\mu = \begin{cases} 0, & \text{for } \pi^0 \text{ along } \ell \\ \vartheta_{\pi^\pm}^\mu, & \text{for } \pi^\pm \text{ along } \ell. \end{cases} \tag{C.8}$$

The twisting angle ϑ_ℓ^μ enters in the denominator but not in the exponential function. We replace $k_\ell^\mu \mapsto k_\ell^\mu - \vartheta_\ell^\mu$ and rewrite the propagator

$$G_\pi(\Delta x_\ell, L) = \sum_{m(\ell)} G_\pi(\Delta x_\ell + Lm(\ell))\, \mathrm{e}^{-i[\Delta x_\ell + Lm(\ell)]\vartheta_\ell}, \tag{C.9}$$

where

$$G_\pi(\Delta x_\ell) = \int \frac{\mathrm{d}^4 k_\ell}{(2\pi)^4} \frac{\mathrm{e}^{ik_\ell \Delta x_\ell}}{M_\pi^2 + k_\ell^2}. \tag{C.10}$$

The propagator is now a sum of propagators in infinite volume without any twisting angles.

We take the product over $\ell \in \mathscr{L}$ and factorize the part of the exponential function depending on $\Delta x_\ell \vartheta_\ell$,

$$\prod_{\ell \in \mathscr{L}} G_\pi(\Delta x_\ell, L) = \mathrm{e}^{-i\sum_{\ell \in \mathscr{L}} \Delta x_\ell \vartheta_\ell} \prod_{\ell \in \mathscr{L}} \sum_{m(\ell)} G_\pi(\Delta x_\ell + Lm(\ell))\, \mathrm{e}^{-iLm(\ell)\vartheta_\ell}. \tag{C.11}$$

The summation $\sum_{\ell \in \mathscr{L}} \Delta x_\ell \vartheta_\ell$ can be evaluated as follows. Without loss of generality we may take $\mathscr{L} = \{\ell_1, \ldots, \ell_N\}$ and consider the graph of Fig. C.1. From the structure of the graph follows

$$\begin{aligned} \sum_{\ell \in \mathscr{L}} \Delta x_\ell \vartheta_\ell &= \sum_{j=1}^{N} [x(f(\ell_j)) - x(i(\ell_j))]\vartheta_{\ell_j} \\ &= -x(i(\ell_1))\vartheta_{\ell_1} + x(i(\ell_2))\underbrace{[\vartheta_{\ell_1} - \vartheta_{\ell_2}]}_{=0} + \cdots + x(i(\ell_{N-1}))\underbrace{[\vartheta_{\ell_{N-2}} - \vartheta_{\ell_{N-1}}]}_{=0} \\ &\quad + x(i(\ell_N))(\vartheta_{\ell_{N-1}} - \vartheta_{\ell_N}) + x(f(\ell_N))\vartheta_{\ell_N}, \end{aligned} \tag{C.12}$$

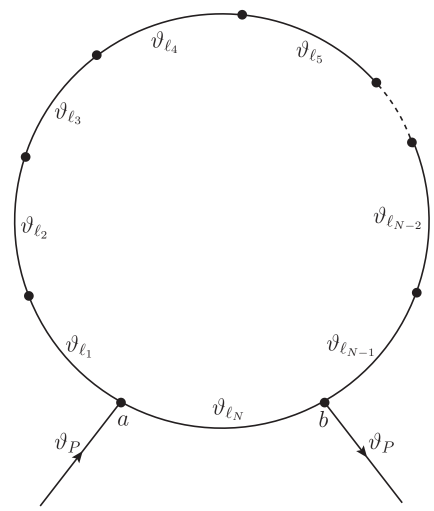


Figure C.1: Auxiliary graph for the sum of internal twisting angles. The endpoints of each line correspond to vertices of $\mathscr{V}$. Along the lines $\ell_1, \ldots, \ell_N$ flow twisting angles $\vartheta^\mu_{\ell_1}, \ldots, \vartheta^\mu_{\ell_N}$. Along external lines flows ϑ^μ_P.

where we use $f(\ell_1) = i(\ell_2), \ldots, f(\ell_{N-1}) = i(\ell_N)$. The square brackets vanish because at each vertex the sum of the twisting angles is zero [36]. This is a consequence of the symmetry constituted by the transformations (2.11). Since $a = i(\ell_1) = f(\ell_N)$ and $b = i(\ell_N)$, we gather the surviving terms

$$\sum_{\ell \in \mathscr{L}} \Delta x_\ell \vartheta_\ell = x(a) \underbrace{(\vartheta_{\ell_N} - \vartheta_{\ell_1})}_{=-\vartheta_P} + x(b) \underbrace{(\vartheta_{\ell_{N-1}} - \vartheta_{\ell_N})}_{=\vartheta_P} = \vartheta_P[x(b) - x(a)]. \tag{C.13}$$

Then, the product of propagators (C.11) may be rewritten as

$$\begin{aligned} \prod_{\ell \in \mathscr{L}} G_\pi(\Delta x_\ell, L) &= \mathrm{e}^{-i\vartheta_P[x(b)-x(a)]} \prod_{\ell \in \mathscr{L}} \sum_{m(\ell)} G_\pi(\Delta x_\ell + Lm(\ell))\, \mathrm{e}^{-iLm(\ell)\vartheta_\ell} \\ &= \mathrm{e}^{-i\vartheta_P[x(b)-x(a)]} \prod_{\ell \in \mathscr{L}} \sum_{n(\ell)} G_\pi(\Delta x_\ell + Ln(\ell) + L\Delta\Lambda_\ell)\, \mathrm{e}^{-iL[n(\ell)+\Delta\Lambda_\ell]\vartheta_\ell}, \end{aligned} \tag{C.14}$$

where in the second equality we transform the gauge field under (C.2) and fix $\Lambda^\mu(b) = 0$. The last exponential function $\exp(-iL\Delta\Lambda_\ell\vartheta_\ell)$ can be factorized and brought to the left side of the product symbol. This yields a summutation $\sum_{\ell\in\mathscr{L}} \Delta\Lambda_\ell\vartheta_\ell$ which can be evaluated in the same way as Eq. (C.13). Recalling that $\Lambda^\mu(b) = 0$ we obtain

$$\prod_{\ell \in \mathscr{L}} G_\pi(\Delta x_\ell, L) = \mathrm{e}^{-i\vartheta_P[x(b)-x(a)-L\Lambda(a)]} \prod_{\ell \in \mathscr{L}} \sum_{n(\ell)} G_\pi(\Delta x_\ell + Ln(\ell) + L\Delta\Lambda_\ell)\, \mathrm{e}^{-iLn(\ell)\vartheta_\ell}. \tag{C.15}$$

We now return to Eq. (C.6) and insert the expression (C.15). We shift the integration variable $x^\mu(v) \mapsto x^\mu(v) - L\Lambda^\mu(v)$ for $v \in \mathscr{V}$ with $\Lambda^\mu(b) = 0$ and interchange the sum over $n^\mu(\ell)$ with products and integrals. The contribution $\mathscr{J}(\mathscr{D}, L)$ becomes a sum over gauge field configurations $\{ n^\mu(\ell) \}$ on $\mathscr{G}$. The sum can be split into two summations [23]. One summation runs over the gauge equivalence classes $[n]$ and the other runs over the gauge transformation $\Lambda^\mu(v)$, $v \in \mathscr{V}$ with $\Lambda^\mu(b) = 0$. As the integrand is periodic in the spatial coordinates the second summation can be combined with the integration over $x^\mu(v)$, $v \in \mathscr{V}'$. Altogether we have,

$$\mathscr{J}(\mathscr{D}, L) = \sum_{[n]} \mathscr{J}(\mathscr{D}, n, L) \tag{C.16a}$$

$$\mathscr{J}(\mathscr{D}, n, L) = \prod_{v \in \mathscr{V}'} \int_{\mathbb{R}^4} \mathrm{d}^4 x(v)\ \mathbb{V} \left\{ \mathrm{e}^{-i(p+\vartheta_P)[x(b)-x(a)]} \prod_{\ell \in \mathscr{L}} G_\pi\left(\Delta x_\ell + Ln(\ell)\right) \mathrm{e}^{-iLn(\ell)\vartheta_\ell} \right\}. \tag{C.16b}$$

We note that the summation over $[n]$ is a well-defined operation. Each term $\mathscr{J}(\mathscr{D}, n, L)$ is gauge invariant and consists of an integration over the whole position space $\mathbb{R}^4$. The term $[n] = [0]$ corresponds to the contribution in infinite volume with the external momentum shifted by ϑ_P^μ,

$$\mathscr{J}(\mathscr{D}, 0, L) = \prod_{v \in \mathscr{V}'} \int_{\mathbb{R}^4} \mathrm{d}^4 x(v)\ \mathbb{V} \left\{ \mathrm{e}^{-i(p+\vartheta_P)[x(b)-x(a)]} \prod_{\ell \in \mathscr{L}} G_\pi\left(\Delta x_\ell\right) \right\}. \tag{C.17}$$

Hence, the contribution of the diagram $\mathscr{D}$ to the self energy $\Delta\Sigma_P = \Sigma_P(L) - \Sigma_P$ is given by the difference

$$\Delta\mathscr{J}(\mathscr{D}) = \mathscr{J}(\mathscr{D}, L) - \mathscr{J}(\mathscr{D}, 0, L) = \sum_{[n] \neq [0]} \mathscr{J}(\mathscr{D}, n, L). \tag{C.18}$$

To determine the behaviour of the self energy at large L we need the heat kernel representation of the propagator,

$$G_\pi\left(\Delta x_\ell + Ln(\ell)\right) = \int_0^\infty \frac{\mathrm{d}t_\ell}{\left(4\pi t_\ell\right)^2}\, \mathrm{e}^{-M_\pi^2 t_\ell - \frac{[\Delta x_\ell + Ln(\ell)]^2}{4t_\ell}}. \tag{C.19}$$

We insert the representation in $\Delta\mathscr{J}(\mathscr{D})$ and perform two substitutions,

$$t_\ell \mapsto \frac{L}{2M_\pi} t_\ell, \quad \text{for } \ell \in \mathscr{L} \tag{C.20a}$$

$$x(v) \mapsto Lx(v), \qquad \text{for } v \in \mathscr{V}'. \tag{C.20b}$$

We take the absolute value and obtain

$$|\Delta\mathscr{J}(\mathscr{D})| \leq \sum_{[n] \neq [0]} \prod_{\ell \in \mathscr{L}} \int_0^\infty \mathrm{d}t_\ell \prod_{v \in \mathscr{V}'} \int_{\mathbb{R}^4} \mathrm{d}^4 x(v)\, L^s\, \frac{|\mathcal{P}_1(t_\ell, x, n)|}{|\mathcal{P}_2(t_\ell)|}\, \mathrm{e}^{-LM_\pi R(t_\ell, x, n, \tilde{E}_P)}, \tag{C.21}$$

where s is some power, $\mathcal{P}_1, \mathcal{P}_2$ are polynomials and

$$R(t_\ell, x, n, \tilde{E}_P) = \tilde{E}_P[x_0(a) - x_0(b)] + \frac{1}{2}\sum_{\ell\in\mathscr{L}}\left\{t_\ell + \frac{[\Delta x_\ell + n(\ell)]^2}{t_\ell}\right\} \tag{C.22}$$

with

$$\tilde{E}_P = \sqrt{\frac{M_P^2}{M_\pi^2} + \frac{|\vec{p} + \vec{\vartheta}_P|^2}{M_\pi^2}} \geq \frac{M_P}{M_\pi} \geq 1. \tag{C.23}$$

The integral (C.21) is of the saddle-point type and for large L can be estimated by expanding around the minimum of the exponent,

$$\begin{aligned} \varepsilon(\mathscr{G}, n) &= \min_{t,x,\tilde{E}_P} R(t_\ell, x, n, \tilde{E}_P) = \min_{t,x} R(t_\ell, x, n, 1) \\ &= \min_x \{\, x_0(a) - x_0(b) + \sum_{\ell\in\mathscr{L}} |\Delta x_\ell + n(\ell)|\,\}\,. \end{aligned} \tag{C.24}$$

Thus, at large L we have

$$\ln[|\Delta\mathscr{J}(\mathscr{D})|] = -LM_\pi\varepsilon(\mathscr{G}, n) + \mathcal{O}(\ln L). \tag{C.25}$$

The next Theorem illustrates the main properties of the minimum $\varepsilon(\mathscr{G}, n)$.

Theorem C.2.1. *Let $\mathscr{C}_1, \ldots, \mathscr{C}_N$ be pairwise disjoint loops in $\mathscr{G}$. Then,*

$$\varepsilon(\mathscr{G}, n) \geq \frac{\sqrt{3}}{2}\sum_{j=1}^{N} |W(\mathscr{C}_j, n)|, \tag{C.26}$$

where $W^\mu(\mathscr{C}, n)$ represents the Wilson loop (C.5). *In particular, if n is not a pure gauge configuration then, $\varepsilon(\mathscr{G}, n) \geq \sqrt{3}/2$.*

Proof. We first prove the claim (C.26) and then the particular case. From Lemma C.1.1 we know that there exists a path $\mathscr{P}$ in $\mathscr{G}$ connecting a, b such that either $\mathscr{P} \cap \mathscr{C}_j = \emptyset$ for all $j = 1, \ldots, N$ or $\mathscr{P} \cap \mathscr{C}_j$ is a path in $\mathscr{G}$ for all $j = 1, \ldots, N$. Note that if $a = b$ one can set $\mathscr{P} = \emptyset$. To every line $\ell \in \mathscr{P}$ one can assign a number $[\mathscr{P} : \ell]$ defined as

$$[\mathscr{P} : \ell] = \begin{cases} 1, & \text{for } \ell \text{ oriented as } \mathscr{P} \\ -1, & \text{otherwise.} \end{cases} \tag{C.27}$$

The number $[\mathscr{P} : \ell]$ satisfies the properties (C.1) of the orientation number and furthermore

$$[\mathscr{P} : \ell] = \begin{cases} 1, & \text{if } i(\ell) = a \\ -1, & \text{if } f(\ell) = a. \end{cases} \tag{C.28}$$

Let $\mathscr{S} \subseteq \mathscr{L}$ be a subset of the line set and $n^\mu(\ell)$ a gauge field on $\mathscr{G}$. We define

$$\epsilon(\mathscr{S}, n) = \min_x \left\{ - \sum_{\ell \in \mathscr{S} \cap \mathscr{P}} [\mathscr{P} : \ell] \Delta x_\ell^0 + \sum_{\ell \in \mathscr{S}} |\Delta x_\ell + n(\ell)| \right\}, \tag{C.29}$$

where $\Delta x_\ell^\mu = x^\mu(f(\ell)) - x^\mu(i(\ell))$. In the case $\mathscr{S} = \emptyset$ we set $\epsilon(\mathscr{S}, n) = 0$. One can show that this quantity satisfies the following relations

$$\epsilon(\mathscr{S}, n) = \varepsilon(\mathscr{G}, n), \qquad \text{if } \mathscr{S} = \mathscr{L} \tag{C.30a}$$

$$\epsilon(\mathscr{S}_1, n) \geq \epsilon(\mathscr{S}_2, n), \qquad \text{if } \mathscr{S}_1 \subset \mathscr{S}_2 \tag{C.30b}$$

$$\epsilon(\mathscr{S}_1 \cup \mathscr{S}_2, n) \geq \epsilon(\mathscr{S}_1, n) + \epsilon(\mathscr{S}_2, n), \qquad \text{if } \mathscr{S}_1 \cap \mathscr{S}_2 = \emptyset. \tag{C.30c}$$

In particular, the relations imply

$$\varepsilon(\mathscr{G}, n) \geq \sum_{j=1}^{N} \epsilon(\mathscr{C}_j, n). \tag{C.31}$$

Now, to prove the claim of Eq. (C.26) remains to show

$$\epsilon(\mathscr{C}_j, n) \geq \frac{\sqrt{3}}{2} |W(\mathscr{C}_j, n)|, \qquad \forall j = 1, \ldots, N. \tag{C.32}$$

We first assume that $\mathscr{P} \cap \mathscr{C}_j = \emptyset$ and consider consecutive vertices $v_1, \ldots, v_M$ along $\mathscr{C}_j$. Then,

$$\epsilon(\mathscr{C}_j, n) = \min_x \left\{ \sum_{k=1}^{M} |x(v_k) - x(v_{k+1}) + [\mathscr{C}_j : \ell_k] n(\ell_k)| \right\}, \tag{C.33}$$

where $v_{M+1} = v_1$ and the line $\ell_k \in \mathscr{C}_j$ has v_k, v_{k+1} as endpoints. We repeatedly use

$$|x_k - x_{k+1} + n| + |x_{k+1} - x_{k+2} + m| \geq |x_k - x_{k+2} + n + m|, \tag{C.34}$$

until we find

$$\epsilon(\mathscr{C}_j, n) \geq \min_x \left\{ |\underbrace{x(v_1) - x(v_{M+1})}_{=0} + \sum_{k=1}^{M} [\mathscr{C}_j : \ell_k] n(\ell_k)| \right\} = |W(\mathscr{C}_j, n)|, \tag{C.35}$$

which is an even stronger inequality than (C.32).

Now, we assume $\mathscr{P} \cap \mathscr{C}_j \neq \emptyset$ and consider consecutive vertices $v_1, \ldots, v_M$ along $\mathscr{C}_j$ with lines $\ell_1, \ldots, \ell_M$ of $\mathscr{C}_j$. As $\mathscr{P} \cap \mathscr{C}_j$ is a path in $\mathscr{G}$ (and hence a path in $\mathscr{C}_j$) it connects two distinct vertices $v_r \neq v_s$. Thus,

$$\epsilon(\mathscr{C}_j, n) = \min_x \left\{ x_0(v_s) - x_0(v_r) + \sum_{k=1}^{M} |x(v_k) - x(v_{k+1}) + [\mathscr{C}_j : \ell_k] n(\ell_k)| \right\}. \tag{C.36}$$

We repeatedly use Eq. (C.34) until we find

$$\epsilon(\mathscr{C}_j, n) \geq \min_{x} \left\{ x_0(v_s) - x_0(v_r) + |x(v_r) - x(v_s)| + \left| x(v_s) - x(v_r) + \underbrace{\sum_{k=1}^{M} [\mathscr{C}_j : \ell_k] n(\ell_k)}_{=W(\mathscr{C}_j, n)} \right| \right\}. \tag{C.37}$$

For convenience, we introduce the short notation

$$\begin{aligned} \mathcal{X}^\mu &= x^\mu(v_s) - x^\mu(v_r) \\ \mathcal{W}^\mu &= W^\mu(\mathscr{C}_j, n), \end{aligned} \tag{C.38}$$

and rewrite the above inequality,

$$\begin{aligned} \epsilon(\mathscr{C}_j, n) &\geq \min_{\mathcal{X}} \{ \mathcal{X}_0 + |\mathcal{X}| + |\mathcal{X} + \mathcal{W}| \} \\ &\geq \min_{\mathcal{X}_0} \{ \mathcal{X}_0 + |\mathcal{X}_0| + |\mathcal{X}_0 + \mathcal{W}| \} \\ &\geq \min_{\mathcal{X}_0} \{ \mathcal{X}_0 + |2\mathcal{X}_0 + \mathcal{W}| \} . \end{aligned} \tag{C.39}$$

We compute the minimum through the differentiation over $\mathcal{X}_0$ and find the inequality (C.32)

$$\begin{aligned} \epsilon(\mathscr{C}_j, n) &\geq \min_{\mathcal{X}_0} \{ \mathcal{X}_0 + \sqrt{4\mathcal{X}_0^2 + \vec{\mathcal{W}}^2} \} \\ &\geq \frac{\sqrt{3}}{2} |\mathcal{W}| = \frac{\sqrt{3}}{2} |W(\mathscr{C}_j, n)|. \end{aligned} \tag{C.40}$$

This concludes the demonstration of the claim of the Theorem,

$$\varepsilon(\mathscr{G}, n) \geq \frac{\sqrt{3}}{2} \sum_{j=1}^{N} |W(\mathscr{C}_j, n)|. \tag{C.41}$$

We now prove the particular case. Let $\mathscr{T}$ be a tree in $\mathscr{G}$ and $n^\mu(\ell)$ its relative axial gauge field. Since $n^\mu(\ell)$ is not a pure gauge field there exists a line $\ell^* \in \mathscr{T}^*$ such that $n^\mu(\ell^*) \neq 0$. For the loop $\mathscr{C}$ with $\mathscr{C} \setminus \{ \ell^* \} \subset \mathscr{T}$, one finds

$$|W(\mathscr{C}, n)| = \left| \sum_{\ell \in \mathscr{L}} [\mathscr{C} : \ell] n(\ell) \right| = |[\mathscr{C} : \ell^*] n(\ell^*)| \geq 1 \tag{C.42}$$

and hence, $\varepsilon(\mathscr{G}, n) \geq \sqrt{3}/2$. □

The next Theorem identifies the class of gauge fields that gives the dominant contribution to $\Delta \mathscr{J}(\mathscr{D})$.

Theorem C.2.2. *Suppose that n is not to a pure gauge configuration and $\varepsilon(\mathscr{G}, n) < \sqrt{3/2}$. Then n is a simple gauge field.*

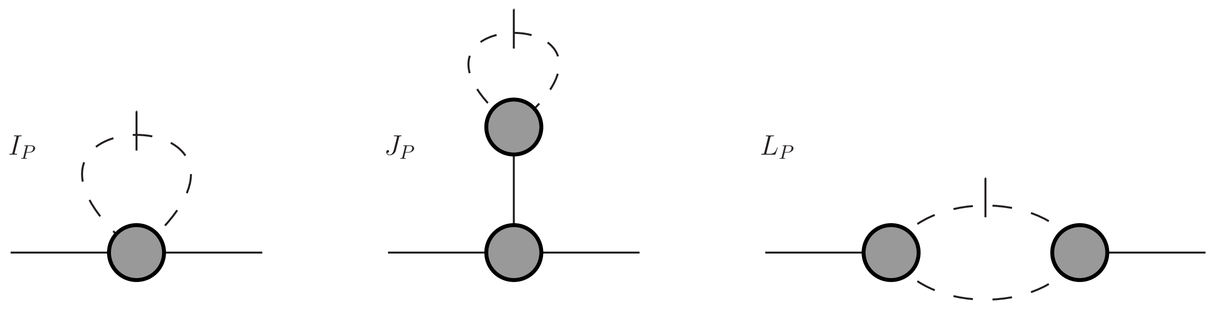


Figure C.2: Skeleton diagrams contributing to the Lüscher formula of a particle P.

We skip the complicated proof of this Theorem (which can be found in Ref. [23]) and show the last steps leading to Eqs. (3.28, 3.58). For all diagrams $\mathscr{D}$ the results of above Theorems can be summarized as

$$\mathscr{J}(\mathscr{D}, n, L) = \mathcal{O}(\mathrm{e}^{-\frac{\sqrt{3}}{2}LM_\pi}), \qquad \text{if } n \text{ is not a pure gauge} \tag{C.43a}$$

$$\Delta\mathscr{J}(\mathscr{D}) = \sum_{[n]\,\text{simple}} \mathscr{J}(\mathscr{D}, n, L) + \mathcal{O}(\mathrm{e}^{-L\bar{M}}), \tag{C.43b}$$

where $\bar{M} \geq \sqrt{3/2}\, M_\pi$. The sum over all diagrams provides the dominant contribution to the self energy

$$\Delta\Sigma_P = \sum_{\mathscr{D}} \sum_{[n]\,\text{simple}} \mathscr{J}(\mathscr{D}, n, L) + \mathcal{O}(\mathrm{e}^{-L\bar{M}}). \tag{C.44}$$

The class of simple gauge fields $[n]$ can be labelled by the set of independent fields (C.4). The self energy becomes

$$\Delta\Sigma_P = \sum_{\mathscr{D}} \sum_{\ell\in\mathscr{D}} \hat{\mathscr{J}}(\mathscr{D}, \ell, L) + \mathcal{O}(\mathrm{e}^{-L\bar{M}}), \tag{C.45}$$

where the second sum runs over all ℓ in $\mathscr{D}$ which belong to at least one loop and which are independent from each other. In momentum space, $\hat{\mathscr{J}}(\mathscr{D}, \ell, L)$ is equal to the integral in infinite volume associated to $\mathscr{D}$ but the momenta are shifted by twisting angles and the integrand is multiplied by

$$\exp[iL\,\vec{n}(\ell, j, \hat{e})\vec{k}_\ell], \tag{C.46}$$

where $\vec{k}_\ell$ is the spatial momentum flowing through ℓ and $\vec{n}(\ell, j, \hat{e})$ is defined in (C.4). These integrals are of the kind represented by the diagrams of Fig. C.2. One can show that the sum (C.45) matches term by term with those diagrams. In the case where P is a pseudoscalar meson the diagrams J_P, L_P are absent. Only the diagram I_P contributes to the self energy

$$\Delta\Sigma_P = \frac{I_P}{2} + \mathcal{O}(\mathrm{e}^{-L\bar{M}}). \tag{C.47}$$

In this case the mass bound can be brought from $\bar{M} = \sqrt{3/2}\, M_\pi$ to $\bar{M} = \sqrt{2}\, M_\pi$, see [32].

C.3 Behaviour of the Matrix Elements of Form Factors at Large L

In a similar way as in Appendix C.2 we can apply Abstract Graph Theory and study the behaviour of the matrix elements of form factors at large volume. We consider two hadrons P, Q in a finite cubic box of the side length L. At the boundaries we impose TBC and redefine the fields so that they are periodic. Let $\mathscr{D}$ be a Feynman diagram contributing to the matrix elements of form factors[2]. To $\mathscr{D}$ we assign the abstract graph $\mathscr{G}$ with the line set $\mathscr{L}$, the vertex set $\mathscr{V}$ and the maps $i, f\colon \mathscr{L} \to \mathscr{V}$. The graph $\mathscr{G}$ is one-particle irreducible and has three external vertices a, b, c, which may coincide. The external momentum p^μ (resp. p'^μ) flows in a (resp. out from b) while $q^\mu = (p'-p)^\mu$ flows in c. The momenta may be additionally shifted by the twisting angle $\vartheta_P^\mu, \vartheta_Q^\mu$ according to the flavor content of P, Q.

In position space, the contribution $\mathscr{J}(\mathscr{D}, L)$ of the diagram $\mathscr{D}$ takes the general form,

$$\mathscr{J}(\mathscr{D}, L) = \prod_{v\in\mathscr{V}'} \int_{\mathbb{R}\times[0,L]^3} \mathrm{d}^4x(v)\ \mathbb{V}\left\{ \mathrm{e}^{i[px(a)-p'x(b)+qx(c)]} \prod_{\ell\in\mathscr{L}} G_\pi\left(\Delta x_\ell, L\right) \right\}. \tag{C.48}$$

Here, $\mathscr{V}' = \mathscr{V} \setminus \{ b \}$ and $\mathbb{V}$ is a product of vertex operators. The product of propagators can be worked out as in Eq. (C.11). We have,

$$\prod_{\ell\in\mathscr{L}} G_\pi\left(\Delta x_\ell, L\right) = \mathrm{e}^{-i\sum_{\ell\in\mathscr{L}}\Delta x_\ell \vartheta_\ell} \prod_{\ell\in\mathscr{L}} \sum_{m(\ell)} G_\pi\left(\Delta x_\ell + Lm(\ell)\right) \mathrm{e}^{-iLm(\ell)\vartheta_\ell}. \tag{C.49}$$

To evaluate the summation $\sum_{\ell\in\mathscr{L}} \Delta x_\ell \vartheta_\ell$ we proceed in a similar way as in Eq. (C.13). We take $\mathscr{L} = \{ \ell_1, \dots, \ell_N \}$ and consider the graph of Fig. C.3. From the structure of the graph follows

$$\begin{aligned}
\sum_{\ell\in\mathscr{L}} \Delta x_\ell \vartheta_\ell &= \sum_{j=1}^{N} [x(f(\ell_j)) - x(i(\ell_j))]\vartheta_{\ell_j} \\
&= -x(i(\ell_1))\vartheta_{\ell_1} + x(i(\ell_2))\underbrace{[\vartheta_{\ell_1} - \vartheta_{\ell_2}]}_{=0} + \dots \\
&\qquad + x(i(\ell_{r+1}))(\vartheta_{\ell_r} - \vartheta_{\ell_{r+1}}) + x(i(\ell_{r+2}))\underbrace{[\vartheta_{\ell_{r+1}} - \vartheta_{\ell_{r+2}}]}_{=0} + \dots \\
&\qquad + x(i(\ell_N))(\vartheta_{\ell_{N-1}} - \vartheta_{\ell_N}) + x(f(\ell_N))\vartheta_{\ell_N},
\end{aligned} \tag{C.50}$$

where we use $f(\ell_1) = i(\ell_2), \dots, f(\ell_{N-1}) = i(\ell_N)$. The square brackets vanish as the sum of the twisting angles at each vertex is zero, see Ref. [36]. Since $a = i(\ell_1) = f(\ell_N)$, $b = i(\ell_N)$, $c = i(\ell_{r+1})$, we gather the surviving terms

$$\sum_{\ell\in\mathscr{L}} \Delta x_\ell \vartheta_\ell = x(a)\underbrace{(\vartheta_{\ell_N} - \vartheta_{\ell_1})}_{=-\vartheta_P} + x(c)\underbrace{(\vartheta_{\ell_r} - \vartheta_{\ell_{r+1}})}_{=\vartheta_P - \vartheta_Q} + x(b)\underbrace{(\vartheta_{\ell_{N-1}} - \vartheta_{\ell_N})}_{=\vartheta_Q}. \tag{C.51}$$

[2]Here, we use the same notation as in Appendix C.2 but the quantities are referred to the matrix elements of form factors.

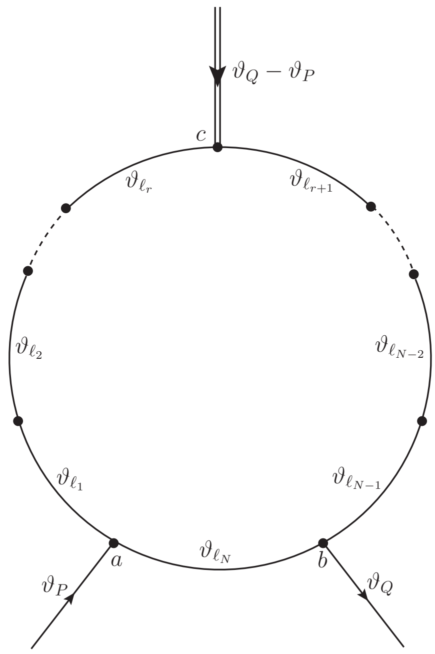


Figure C.3: Auxiliary graph for the sum of internal twisting angles.

The product of propagators becomes

$$\prod_{\ell\in\mathscr{L}} G_\pi\left(\Delta x_\ell, L\right) = \mathrm{e}^{i\left[x(a)\vartheta_P - x(b)\vartheta_Q + x(c)(\vartheta_P-\vartheta_Q)\right]} \prod_{\ell\in\mathscr{L}} \sum_{m(\ell)} G_\pi\left(\Delta x_\ell + Lm(\ell)\right)\, \mathrm{e}^{-iLm(\ell)\vartheta_\ell}. \tag{C.52}$$

We can further work out the product of propagators if we transform the gauge field under (C.2) and fix $\Lambda^\mu(b) = 0$. This yields an exponential function $\exp(-iL\Delta\Lambda_\ell\vartheta_\ell)$ that can be factorized and evaluated in the same way as Eq. (C.51). The product of propagators becomes

$$\begin{aligned}\prod_{\ell\in\mathscr{L}} G_\pi\left(\Delta x_\ell, L\right) = {} & \mathrm{e}^{i\left[x(a)\vartheta_P - x(b)\vartheta_Q + x(c)(\vartheta_P-\vartheta_Q)\right]}\mathrm{e}^{i\left[L\Lambda(a)\vartheta_P + L\Lambda(c)(\vartheta_Q-\vartheta_P)\right]} \\ & \times \prod_{\ell\in\mathscr{L}} \sum_{n(\ell)} G_\pi\left(\Delta x_\ell + Ln(\ell) + L\Delta\Lambda_\ell\right)\, \mathrm{e}^{-iLn(\ell)\vartheta_\ell}.\end{aligned} \tag{C.53}$$

We insert this expression in Eq. (C.48) and shift the integration variable $x^\mu(v) \mapsto x^\mu(v) - L\Lambda^\mu(v)$ for $v \in \mathscr{V}$ with $\Lambda^\mu(b) = 0$. Then, we interchange the sum over $n^\mu(\ell)$ with products and integrals. The contribution $\mathscr{J}(\mathscr{D}, L)$ becomes a sum over gauge field configurations $\{\, n^\mu(\ell)\,\}$ on $\mathscr{G}$. The sum can be split into a summation over $[n]$ and a summation over $\Lambda^\mu(v)$, $v \in \mathscr{V}$ with $\Lambda^\mu(b) = 0$. Due to the periodicity of the integrand the second summation can be combined with the integration over $x^\mu(v)$, $v \in \mathscr{V}'$. Altogether, we have

$$\mathscr{J}(\mathscr{D}, L) = \sum_{[n]} \mathscr{J}(\mathscr{D}, n, L) \tag{C.54a}$$

$$\mathscr{J}(\mathscr{D}, n, L) = \prod_{v\in\mathscr{V}'} \int_{\mathbb{R}^4} \mathrm{d}^4 x(v)\ \mathbb{V}\Bigg\{ \mathrm{e}^{i\left[x(a)(p+\vartheta_P)-x(b)(p'+\vartheta_Q)+x(c)(q+\vartheta_Q-\vartheta_P)\right]} \times \prod_{\ell\in\mathscr{L}} G_\pi\left(\Delta x_\ell + Ln(\ell)\right) \mathrm{e}^{-iLn(\ell)\vartheta_\ell} \Bigg\}. \tag{C.54b}$$

The contribution $\mathscr{J}(\mathscr{D}, L)$ is now expressed as a summation over $[n]$ of gauge invariant terms. The term $[n] = [0]$ corresponds to the contribution in infinite volume with external momenta shifted by $\vartheta_P^\mu, \vartheta_Q^\mu$,

$$\mathscr{J}(\mathscr{D}, 0, L) = \prod_{v\in\mathscr{V}'} \int_{\mathbb{R}^4} \mathrm{d}^4 x(v)\ \mathbb{V}\left\{ \mathrm{e}^{i\left[x(a)(p+\vartheta_P)-x(b)(p'+\vartheta_Q)+x(c)(q+\vartheta_Q-\vartheta_P)\right]} \prod_{\ell\in\mathscr{L}} G_\pi\left(\Delta x_\ell\right) \right\}. \tag{C.55}$$

Hence, the contribution of the diagram $\mathscr{D}$ to the corrections of the matrix elements of form factors is given by the difference,

$$\Delta\mathscr{J}(\mathscr{D}) = \mathscr{J}(\mathscr{D}, L) - \mathscr{J}(\mathscr{D}, 0, L) = \sum_{[n]\neq[0]} \mathscr{J}(\mathscr{D}, n, L). \tag{C.56}$$

By means of the heat kernel representation (C.19) and of the substitutions (C.20) we can estimate the absolute value,

$$|\Delta\mathscr{J}(\mathscr{D})| \leq \sum_{[n]\neq[0]} \prod_{\ell\in\mathscr{L}} \int_0^\infty \mathrm{d}t_\ell \prod_{v\in\mathscr{V}'} \int_{\mathbb{R}^4} \mathrm{d}^4 x(v)\, L^s \frac{|\mathcal{P}_1(t_\ell, x, n)|}{|\mathcal{P}_2(t_\ell)|} \mathrm{e}^{-LM_\pi R(t_\ell, x, n, \tilde{E}_P, \tilde{E}_Q)}. \tag{C.57}$$

Here, s is some power, $\mathcal{P}_1, \mathcal{P}_2$ are polynomials and

$$R(t_\ell, x, n, \tilde{E}_P, \tilde{E}_Q) = \tilde{E}_P[x_0(a) - x_0(c)] + \tilde{E}_Q[x_0(c) - x_0(b)] + \frac{1}{2}\sum_{\ell\in\mathscr{L}} \left\{ t_\ell + \frac{\left[\Delta x_\ell + n(\ell)\right]^2}{t_\ell} \right\} \tag{C.58}$$

with

$$\tilde{E}_P = \sqrt{\frac{M_P^2}{M_\pi^2} + \frac{|\vec{p} + \vec{\vartheta}_P|^2}{M_\pi^2}} \geq \frac{M_P}{M_\pi} \geq 1 \tag{C.59a}$$

$$\tilde{E}_Q = \sqrt{\frac{M_Q^2}{M_\pi^2} + \frac{|\vec{p} + \vec{\vartheta}_Q|^2}{M_\pi^2}} \geq \frac{M_Q}{M_\pi} \geq 1. \tag{C.59b}$$

The integral (C.57) is of the saddle-point type and for large L can be estimated by expanding around the minimum of the exponent,

$$\begin{aligned}\varepsilon(\mathscr{G},n) &= \min_{t,x,\tilde{E}_P,\tilde{E}_Q} R(t_\ell,x,n,\tilde{E}_P,\tilde{E}_Q) = \min_{t,x} R(t_\ell,x,n,1,1) \\ &= \min_{x} \{\, x_0(a) - x_0(b) + \sum_{\ell\in\mathscr{L}} |\Delta x_\ell + n(\ell)| \,\} \,.\end{aligned} \tag{C.60}$$

Thus, at large L we have

$$\ln[|\Delta\mathscr{J}(\mathscr{D})|] = -LM_\pi \varepsilon(\mathscr{G},n) + \mathcal{O}(\ln L). \tag{C.61}$$

Note that the minimum $\varepsilon(\mathscr{G},n)$ is exactly the same as in the case of the self energy, see Eq. (C.24). Hence, we can apply the Theorems C.2.1 and C.2.2 without any modifications. The result is that for all diagrams $\mathscr{D}$,

$$\mathscr{J}(\mathscr{D},n,L) = \mathcal{O}(\mathrm{e}^{-\frac{\sqrt{3}}{2}LM_\pi}), \qquad \text{if } n \text{ is not a pure gauge} \tag{C.62a}$$

$$\Delta\mathscr{J}(\mathscr{D}) = \sum_{[n]\,\text{simple}} \mathscr{J}(\mathscr{D},n,L) + \mathcal{O}(\mathrm{e}^{-L\bar{M}}), \tag{C.62b}$$

where $\bar{M} \geq \sqrt{3/2}\,M_\pi$. The sum over all diagrams provides the dominant contribution to the corrections of the matrix elements of form factors.

Appendix D

Terms $S^{(4)}$

We list the explicit expressions of the terms $S^{(4)}$ introduced in Chapter 4. Some of them are parts of the terms $S^{(4)}_{M_P}, S^{(4)}_{F_P}$ presented in Appendix A of Ref. [32]; others are completely new. For completeness, we list them all and for each of them we indicate the equation they appear.

D.1 Pions

We begin with the terms $S^{(4)}$ appearing in the asymptotic formulae for pions. Remark that the functions $R_0^k, (R_0^k)', (R_0^k)'', Q_0^k, (Q_0^k)'$ are defined in Eq. (D.17).
The terms appearing in Eq. (4.55) are

$$\begin{aligned} S^{(4)}(M_{\pi^0}, \pi^0) &= 3R_0^0 - 8R_0^1 - 8R_0^2 \\ S^{(4)}(M_{\pi^0}, \pi^\pm) &= \frac{4}{3}\left(R_0^0 + 2R_0^1 - 4R_0^2\right). \end{aligned} \tag{D.1}$$

The terms appearing in Eq. (4.61) are

$$\begin{aligned} S^{(4)}(M_{\pi^\pm}, \pi^0) &= \frac{2}{3}\left(R_0^0 + 2R_0^1 - 4R_0^2\right) \\ S^{(4)}(M_{\pi^\pm}, \pi^\pm) &= \frac{1}{3}\left(11R_0^0 - 20R_0^1 - 32R_0^2\right). \end{aligned} \tag{D.2}$$

The terms appearing in Eq. (4.63) are

$$\begin{aligned} S_D^{(4)}(M_{\pi^\pm}, \pi^0) &= \frac{4}{3}\left(R_0^1 - 4R_0^2\right) - \frac{4}{3}\left[(R_0^1)' - 2(R_0^2)' - 4(R_0^3)'\right] \\ S_D^{(4)}(M_{\pi^\pm}, \pi^\pm) &= -\frac{4}{3}\left(5R_0^1 + 16R_0^2\right) - \frac{2}{3}\left[11(R_0^1)' + 20(R_0^2)' - 32(R_0^3)'\right]. \end{aligned} \tag{D.3}$$

The term appearing in Eq. (4.66) is

$$S^{(4)}(\vartheta_{\Sigma_{\pi^+}}) = -\frac{1}{3}\left(11R_0^1 + 20R_0^2 - 8R_0^3\right). \tag{D.4}$$

The terms appearing in Eq. (4.70) are

$$\begin{aligned} S^{(4)}(F_{\pi^0},\pi^0) &= -4\left(R_0^1+2R_0^2\right)-\frac{1}{2}\left[3(R_0^0)'-8(R_0^1)'-8(R_0^2)'\right] \\ S^{(4)}(F_{\pi^0},\pi^\pm) &= \frac{4}{3}\left(R_0^0+2R_0^1-4R_0^2\right)-\frac{2}{3}\left[(R_0^0)'+2(R_0^1)'-4(R_0^2)'\right]. \end{aligned} \tag{D.5}$$

The terms appearing in Eq. (4.74) are

$$\begin{aligned} S^{(4)}(F_{\pi^\pm},\pi^0) &= \frac{2}{3}\left(R_0^0+2R_0^1-4R_0^2\right)-\frac{1}{3}\left[(R_0^0)'+2(R_0^1)'-4(R_0^2)'\right] \\ S^{(4)}(F_{\pi^\pm},\pi^\pm) &= \frac{2}{3}\left(R_0^0-4R_0^1-16R_0^2\right)-\frac{1}{6}\left[11(R_0^0)'-20(R_0^1)'-32(R_0^2)'\right]. \end{aligned} \tag{D.6}$$

The terms appearing in Eq. (4.75) are

$$\begin{aligned} S_D^{(4)}(F_{\pi^\pm},\pi^0) &= \frac{4}{3}\left(R_0^1-4R_0^2\right)-\frac{2}{3}\left[3(R_0^1)'-8(R_0^2)'-8(R_0^3)'\right] \\ &\qquad +\frac{2}{3}\left[(R_0^1)''-2(R_0^2)''-4(R_0^3)''\right] \\ S_D^{(4)}(F_{\pi^\pm},\pi^\pm) &= -\frac{8}{3}\left(R_0^1+8R_0^2\right)+\frac{2}{3}\left[3(R_0^1)'+8(R_0^2)'+32(R_0^3)'\right] \\ &\qquad +\frac{1}{3}\left[11(R_0^1)''+20(R_0^2)''-32(R_0^3)''\right]. \end{aligned} \tag{D.7}$$

The term appearing in Eq. (4.78) is

$$S^{(4)}(\vartheta_{\mathscr{A}_{\pi^+}}) = -\frac{2}{3}\left(R_0^1+4R_0^2-4R_0^3\right)+\frac{1}{6}\left[11(R_0^1)'+20(R_0^2)'-8(R_0^3)'\right]. \tag{D.8}$$

The terms appearing in Eq. (4.82) are

$$\begin{aligned} S^{(4)}(G_{\pi^0},\pi^0) &= -3R_0^0+4R_0^1-\frac{1}{2}\left[3(R_0^0)'-8(R_0^1)'-8(R_0^2)'\right] \\ S^{(4)}(G_{\pi^0},\pi^\pm) &= -\frac{2}{3}\left[(R_0^0)'+2(R_0^1)'-4(R_0^2)'\right]. \end{aligned} \tag{D.9}$$

The terms appearing in Eq. (4.88) are

$$\begin{aligned} S^{(4)}(G_{\pi^\pm},\pi^0) &= -\frac{1}{3}\left[(R_0^0)'+2(R_0^1)'-4(R_0^2)'\right] \\ S^{(4)}(G_{\pi^\pm},\pi^\pm) &= -3R_0^0+4R_0^1-\frac{1}{6}\left[11(R_0^0)'-20(R_0^1)'-32(R_0^2)'\right]. \end{aligned} \tag{D.10}$$

The terms appearing in Eq. (4.89) are

$$\begin{aligned} S_D^{(4)}(G_{\pi^\pm},\pi^0) &= -\frac{2}{3}\left[(R_0^1)'-4(R_0^2)'-(R_0^1)''+2(R_0^2)''+4(R_0^3)''\right] \\ S_D^{(4)}(G_{\pi^\pm},\pi^\pm) &= 4R_0^1+\frac{28}{3}\left[(R_0^1)'+2(R_0^2)'\right]+\frac{1}{3}\left[11(R_0^1)''+20(R_0^2)''-32(R_0^3)''\right]. \end{aligned} \tag{D.11}$$

The term appearing in Eq. (4.92) is

$$S^{(4)}(\vartheta_{\mathscr{G}_{\pi^+}}) = 3R_0^1 + 4R_0^2 + \frac{1}{6}\left[11(R_0^1)' + 20(R_0^2)' - 8(R_0^3)'\right]. \tag{D.12}$$

The terms appearing in Eq. (4.98) are

$$\begin{aligned} S^{(4)}(\Gamma_S^{\pi^0}, \pi^0) &= 5\left(3R_0^0 - 8R_0^1 - 8R_0^2\right) - (3Q_0^0 - 8Q_0^1 - 8Q_0^2) \\ S^{(4)}(\Gamma_S^{\pi^0}, \pi^\pm) &= \frac{20}{3}\left(R_0^0 + 2R_0^1 - 4R_0^2\right) - \frac{4}{3}\left(Q_0^0 + 2Q_0^1 - 4Q_0^2\right). \end{aligned} \tag{D.13}$$

The terms appearing in Eq. (4.102) are

$$\begin{aligned} S^{(4)}(\Gamma_S^{\pi^\pm}, \pi^0) &= \frac{10}{3}\left(R_0^0 + 2R_0^1 - 4R_0^2\right) - \frac{2}{3}\left(Q_0^0 + 2Q_0^1 - 4Q_0^2\right) \\ S^{(4)}(\Gamma_S^{\pi^\pm}, \pi^\pm) &= \frac{5}{3}\left(11R_0^0 - 20R_0^1 - 32R_0^2\right) - \frac{1}{3}\left(11Q_0^0 - 20Q_0^1 - 32Q_0^2\right). \end{aligned} \tag{D.14}$$

The terms appearing in Eq. (4.103) are

$$\begin{aligned} S_D^{(4)}(\Gamma_S^{\pi^\pm}, \pi^0) &= \frac{4}{3}[4 - C_{\pi^\pm}]\left[R_0^1 - 4R_0^2 - (R_0^1)' + 2(R_0^2)' + 4(R_0^3)'\right] \\ &\quad - \frac{4}{3}\left[Q_0^1 - 4Q_0^2 - (Q_0^1)' + 2(Q_0^2)' + 4(Q_0^3)'\right] \\ S_D^{(4)}(\Gamma_S^{\pi^\pm}, \pi^\pm) &= -\frac{2}{3}[4 - C_{\pi^\pm}]\left[10R_0^1 + 32R_0^2 + 11(R_0^1)' + 20(R_0^2)' - 32(R_0^3)'\right] \\ &\quad + \frac{2}{3}\left[10Q_0^1 + 32Q_0^2 + 11(Q_0^1)' + 20(Q_0^2)' - 32(Q_0^3)'\right]. \end{aligned} \tag{D.15}$$

Here, $C_{\pi^\pm} = M_\pi/(M_\pi + D_{\pi^\pm})$ and $D_{\pi^\pm} = \sqrt{M_\pi^2 + |\vec{\vartheta}_{\pi^\pm}|^2} - M_\pi$.
The term appearing in Eq. (4.104) is

$$S_{\Gamma_S}^{(4)}(\Theta_{\pi^+}) = -\frac{5}{3}\left(11R_0^1 + 20R_0^2 - 8R_0^3\right) + \frac{1}{3}\left(11Q_0^1 + 20Q_0^2 - 8Q_0^3\right). \tag{D.16}$$

The functions $R_0^k, (R_0^k)', (R_0^k)'', Q_0^k, (Q_0^k)'$ entering the above expressions are defined as

$$
\begin{aligned}
R_0^k &= R_0^k(\lambda_\pi|\vec{n}|) \\
&= \begin{cases} \mathrm{Re} \\ \mathrm{Im} \end{cases} \int_{\mathbb{R}} \mathrm{d}y\, y^k \mathrm{e}^{-\lambda_\pi|\vec{n}|\sqrt{1+y^2}} g(2+2iy), \qquad \text{for} \quad \begin{cases} k \text{ even} \\ k \text{ odd} \end{cases} \\
(R_0^k)' &= (R_0^k)'(\lambda_\pi|\vec{n}|) \\
&= \begin{cases} \mathrm{Re} \\ \mathrm{Im} \end{cases} \int_{\mathbb{R}} \mathrm{d}y\, y^k \mathrm{e}^{-\lambda_\pi|\vec{n}|\sqrt{1+y^2}} g'(2+2iy), \qquad \text{for} \quad \begin{cases} k \text{ even} \\ k \text{ odd} \end{cases} \\
(R_0^k)'' &= (R_0^k)''(\lambda_\pi|\vec{n}|) \\
&= \begin{cases} \mathrm{Re} \\ \mathrm{Im} \end{cases} \int_{\mathbb{R}} \mathrm{d}y\, y^k \mathrm{e}^{-\lambda_\pi|\vec{n}|\sqrt{1+y^2}} g''(2+2iy), \qquad \text{for} \quad \begin{cases} k \text{ even} \\ k \text{ odd,} \end{cases} \\
Q_0^k &= Q_0^k(\lambda_\pi|\vec{n}|) \\
&= \begin{cases} \mathrm{Re} \\ \mathrm{Im} \end{cases} \int_{\mathbb{R}} \mathrm{d}y\, y^k \lambda_\pi|\vec{n}|\sqrt{1+y^2}\mathrm{e}^{-\lambda_\pi|\vec{n}|\sqrt{1+y^2}} g(2+2iy), \qquad \text{for} \quad \begin{cases} k \text{ even} \\ k \text{ odd} \end{cases} \\
(Q_0^k)' &= (Q_0^k)'(\lambda_\pi|\vec{n}|) \\
&= \begin{cases} \mathrm{Re} \\ \mathrm{Im} \end{cases} \int_{\mathbb{R}} \mathrm{d}y\, y^k \lambda_\pi|\vec{n}|\sqrt{1+y^2}\mathrm{e}^{-\lambda_\pi|\vec{n}|\sqrt{1+y^2}} g'(2+2iy), \qquad \text{for} \quad \begin{cases} k \text{ even} \\ k \text{ odd} \end{cases}
\end{aligned}
\tag{D.17}
$$

where

$$
\begin{aligned}
g(x) &= \sigma \log\left(\frac{\sigma-1}{\sigma+1}\right) + 2 \\
\sigma &= \sqrt{1-4/x},
\end{aligned}
\tag{D.18}
$$

and $g'(x)$, $g''(x)$ are the first and second derivative of $g(x)$ with respect to x. Note that $g(x)$ is related to the loop-integral function $\bar{J}(q^2) = J(q^2) - J(0)$ evaluated in $d = 4$ dimensions,

$$
J(q^2) = \int \frac{\mathrm{d}^d k}{(2\pi)^d} \frac{1}{i\,[M_\pi^2 - (k+q)^2]\,[M_\pi^2 - k^2]}, \tag{D.19}
$$

according to $g(x) = (4\pi)^2\, \bar{J}(xM_\pi^2)$.

D.2 Kaons

We list the terms $S^{(4)}$ appearing in the asymptotic formulae for kaons. Remark that the functions S^{kl}_{PQ} are defined in Eq. (D.30). In the next expressions, we denote the ratio of mass squares as $x_{PQ} = M_P^2/M_Q^2$ where $P, Q = \pi, K, \eta$.
The term appearing in Eq. (4.109) is

$$\begin{aligned} S^{(4)}(M_{K^\pm}, \pi^\pm) = 2x_{\pi K}^{-1/2} \Big\{ & + \frac{3}{32}(1+x_{\pi K})^2 S^{0,1}_{K\pi} - \frac{5}{8}(1+x_{K\pi}) S^{1,1}_{K\pi} - \frac{19}{8} S^{2,1}_{K\pi} \\ & - \frac{3}{16}(1-x_{\pi K}^2) S^{0,3}_{K\pi} \\ & + \frac{13}{8}(1-x_{\pi K}) S^{1,3}_{K\pi} - \frac{3}{2}\left(x_{\pi K}\, S^{0,5}_{K\pi} + S^{2,5}_{K\pi}\right) \\ & + \frac{1}{96}(1+x_{\pi K})^2 S^{0,1}_{\eta K} - \frac{1}{8}(1+x_{\pi K}) S^{1,1}_{\eta K} - \frac{3}{8} S^{2,1}_{\eta K} \\ & - \frac{1}{16}(1+x_{\pi K})\,(5-2x_{\pi K}-3x_{\eta K})\, S^{0,3}_{\eta K} \\ & + \frac{3}{8}\,(1-2x_{\pi K}+x_{\eta K})\, S^{1,3}_{\eta K} - \frac{3}{2}\left(x_{\pi K}\, S^{0,5}_{\eta K} + S^{2,5}_{\eta K}\right) \Big\}. \end{aligned} \tag{D.20}$$

The term appearing in Eq. (4.111) is

$$\begin{aligned} S^{(4)}_D(M_{K^\pm}, \pi^\pm) = 2x_{\pi K}^{-1/2} \Big\{ & - \frac{5}{8}(1+x_{\pi K}) S^{1,1}_{K\pi} - \frac{3}{16}(1+x_{\pi K})^2 S^{1,2}_{K\pi} \\ & + \frac{13}{8}(1-x_{\pi K}) S^{1,3}_{K\pi} \\ & + \frac{3}{8}(1-x_{\pi K}^2) S^{1,4}_{K\pi} - \frac{19}{4}(S^{2,1}_{K\pi} - S^{3,2}_{K\pi}) \\ & - \frac{5}{4}(1+x_{\pi K}) S^{2,2}_{K\pi} + \frac{13}{4}(1-x_{\pi K}) S^{2,4}_{K\pi} \\ & + 3\left(x_{\pi K} S^{1,6}_{K\pi} - S^{2,5}_{K\pi} + S^{3,6}_{K\pi}\right) \\ & - \frac{1}{8}(1+x_{\pi K}) S^{1,1}_{\eta K} - \frac{1}{48}(1+x_{\pi K})^2 S^{1,2}_{\eta K} \\ & + \frac{3}{8}(1-2x_{\pi K}+x_{\eta K}) S^{1,3}_{\eta K} \\ & + \frac{1}{8}(1+x_{\pi K})\,(5-2x_{\pi K}-3x_{\eta K})\, S^{1,4}_{\eta K} - \frac{3}{4}\left(S^{2,1}_{\eta K} - S^{3,2}_{\eta K}\right) \\ & - \frac{1}{4}(1+x_{\pi K}) S^{2,2}_{\eta K} + \frac{3}{4}(1-2x_{\pi K}+x_{\eta K}) S^{2,4}_{\eta K} \\ & + 3\left(x_{\pi K}\, S^{1,6}_{\eta K} - S^{2,5}_{\eta K} + S^{3,6}_{\eta K}\right) \Big\}. \end{aligned} \tag{D.21}$$

The term appearing in Eq. (4.114) is

$$
\begin{aligned}
S^{(4)}(\vartheta_{\Sigma_{K^+}}) = x_{\pi K}^{-1}\Big\{ & -\frac{3}{16}(1+x_{\pi K})^2 S_{K\pi}^{1,1} + \frac{3}{8}(1-x_{\pi K}^2) S_{K\pi}^{1,3} \\
& - \frac{5}{4}(1+x_{\pi K}) S_{K\pi}^{2,1} + \frac{13}{4}(1-x_{\pi K}) S_{K\pi}^{2,3} + \frac{3}{4} S_{K\pi}^{3,1} \\
& + 3\left(x_{\pi K}\, S_{K\pi}^{1,5} + S_{K\pi}^{3,5}\right) \\
& - \frac{1}{48}(1+x_{\pi K})^2 S_{\eta K}^{1,1} + \frac{1}{8}(1+x_{\pi K})\left(5-2x_{\pi K}-3x_{\eta K}\right) S_{\eta K}^{1,3} \\
& - \frac{1}{4}(1+x_{\pi K}) S_{\eta K}^{2,1} + \frac{3}{4}(1-2x_{\pi K}+x_{\eta K}) S_{\eta K}^{2,3} + \frac{3}{4} S_{\eta K}^{3,1} \\
& + 3\left(x_{\pi K} S_{\eta K}^{1,5} + S_{\eta K}^{3,5}\right)\Big\}.
\end{aligned}
\tag{D.22}
$$

The term appearing in Eq. (4.118) is

$$
\begin{aligned}
S^{(4)}(F_{K^\pm}, \pi^\pm) = 2\, x_{\pi K}^{-1/2}\Big\{ & -\frac{5}{16}(1+x_{\pi K}) S_{K\pi}^{1,1} - \frac{3}{64}(1+x_{\pi K})^2 S_{K\pi}^{0,2} \\
& + \frac{5}{16}(1+x_{\pi K}) S_{K\pi}^{1,2} + \frac{3}{32}\left(1-5x_{\pi K}\right) S_{K\pi}^{0,3} \\
& + \frac{1}{8}\left(16-5x_{\pi K}\right) S_{K\pi}^{1,3} + \frac{5}{4} S_{K\pi}^{2,3} \\
& + \frac{3}{32}\left(1-x_{\pi K}^2\right) S_{K\pi}^{0,4} \\
& - \frac{13}{16}(1-x_{\pi K}) S_{K\pi}^{1,4} - \frac{19}{16}\left(2\, S_{K\pi}^{2,1} - S_{K\pi}^{2,2}\right) \\
& - \frac{3}{4}\left(x_{\pi K}\, S_{K\pi}^{0,5} + 2\, S_{K\pi}^{2,5} - x_{\pi K}\, S_{K\pi}^{0,6} - S_{K\pi}^{2,6}\right) \\
& - \frac{1}{16}(1+x_{\pi K}) S_{\eta K}^{1,1} - \frac{1}{192}(1+x_{\pi K})^2 S_{\eta K}^{0,2} \\
& + \frac{1}{16}(1+x_{\pi K}) S_{\eta K}^{1,2} - \frac{1}{32}\left(11+2x_{\pi K}-9x_{\eta K}\right) S_{\eta K}^{0,3} \\
& + \frac{1}{8}(4-2x_{\pi K}+3x_{\eta K}) S_{\eta K}^{1,3} + \frac{3}{4} S_{\eta K}^{2,3} \\
& + \frac{1}{32}(1+x_{\pi K})\left(5-2x_{\pi K}-3x_{\eta K}\right) S_{\eta K}^{0,4} \\
& - \frac{3}{16}(1-2x_{\pi K}+x_{\eta K}) S_{\eta K}^{1,4} - \frac{3}{16}\left(2\, S_{\eta K}^{2,1} - S_{\eta K}^{2,2}\right) \\
& - \frac{3}{4}\left(x_{\pi K}\, S_{\eta K}^{0,5} + 2\, S_{\eta K}^{2,5} - x_{\pi K}\, S_{\eta K}^{0,6} - S_{\eta K}^{2,6}\right)\Big\}.
\end{aligned}
\tag{D.23}
$$

The term appearing in Eq. (4.120) is

$$
\begin{aligned}
S_D^{(4)}(F_{K^\pm},\pi^\pm) = 2\,x_{\pi K}^{-1/2}\Big\{ & -\frac{5}{16}(1+x_{\pi K})S_{K\pi}^{1,1} + \frac{5}{16}(1+x_{\pi K})S_{K\pi}^{1,2} \\
& + \frac{1}{8}(16-5x_{\pi K})S_{K\pi}^{1,3} - \frac{1}{4}(4-7x_{\pi K})S_{K\pi}^{1,4} \\
& + \frac{3}{32}(1+x_{\pi K})^2 S_{K\pi}^{1,7} \\
& - \frac{3}{16}(1-x_{\pi K}^2)S_{K\pi}^{1,8} \\
& + \frac{1}{8}(14-5x_{\pi K})S_{K\pi}^{2,2} + \frac{1}{4}\left(16-5x_{\pi K}\right)S_{K\pi}^{2,4} \\
& + \frac{5}{8}(1+x_{\pi K})S_{K\pi}^{2,7} - \frac{13}{8}(1-x_{\pi K})S_{K\pi}^{2,8} \\
& + \frac{3}{2}\left(x_{\pi K}\,S_{K\pi}^{1,6} - x_{\pi K}\,S_{K\pi}^{1,9} + S_{K\pi}^{2,6} - S_{K\pi}^{3,9}\right) \\
& - \frac{19}{8}\left(2\,S_{K\pi}^{2,1} - 2\,S_{K\pi}^{3,2} + S_{K\pi}^{3,7}\right) \\
& + \frac{5}{2}\left(S_{K\pi}^{2,3} - S_{K\pi}^{3,4}\right) - 3\left(S_{K\pi}^{2,5} - S_{K\pi}^{3,6}\right) \\
& - \frac{1}{16}(1+x_{\pi K})S_{\eta K}^{1,1} + \frac{1}{16}(1+x_{\pi K})S_{\eta K}^{1,2} \\
& + \frac{1}{8}(4-2x_{\pi K}+3x_{\eta K})S_{\eta K}^{1,3} + \frac{1}{4}(2+2x_{\pi K}-3x_{\eta K})S_{\eta K}^{1,4} \\
& + \frac{1}{96}(1+x_{\pi K})^2 S_{\eta K}^{1,7} \\
& - \frac{1}{16}(1+x_{\pi K})\left(5-2x_{\pi K}-3x_{\eta K}\right)S_{\eta K}^{1,8} \\
& + \frac{1}{8}(2-x_{\pi K})S_{\eta K}^{2,2} + \frac{1}{4}(4-2x_{\pi K}+3x_{\eta K})S_{\eta K}^{2,4} \\
& + \frac{1}{8}(1+x_{\pi K})S_{\eta K}^{2,7} - \frac{3}{8}(1-2x_{\pi K}+x_{\eta K})S_{\eta K}^{2,8} \\
& + \frac{3}{2}\left(x_{\pi K}\,S_{\eta K}^{1,6} - x_{\pi K}\,S_{\eta K}^{1,9} + S_{\eta K}^{2,6} - S_{\eta K}^{3,9}\right) \\
& - \frac{3}{8}\left(2\,S_{\eta K}^{2,1} - 2\,S_{\eta K}^{3,2} + S_{\eta K}^{3,7}\right) \\
& + \frac{3}{2}\left(S_{\eta K}^{2,3} - S_{\eta K}^{3,4}\right) - 3\left(S_{\eta K}^{2,5} - S_{\eta K}^{3,6}\right)\Big\}.
\end{aligned}
\tag{D.24}
$$

The term appearing in Eq. (4.123) is

$$
\begin{aligned}
S^{(4)}(\vartheta_{\mathscr{A}_{K^+}}) = x_{\pi K}^{-1}\Big\{ &+ \frac{3}{32}(1+x_{\pi K})^2 S_{K\pi}^{1,2} - \frac{3}{16}(1-5x_{\pi K})S_{K\pi}^{1,3} \\
&- \frac{3}{16}(1-x_{\pi K}^2)S_{K\pi}^{1,4} - \frac{5}{8}(1+x_{\pi K})S_{K\pi}^{2,1} \\
&+ \frac{5}{8}(1+x_{\pi K})S_{K\pi}^{2,2} + \frac{1}{4}(16-5x_{\pi K})S_{K\pi}^{2,3} \\
&- \frac{13}{8}(1-x_{\pi K})S_{K\pi}^{2,4} + \frac{3}{4}S_{K\pi}^{3,1} - \frac{3}{8}S_{K\pi}^{3,2} \\
&- \frac{5}{2}S_{K\pi}^{3,3} + 3\,S_{K\pi}^{3,5} \\
&+ \frac{3}{2}\left(x_{\pi K}\,S_{K\pi}^{1,5} - x_{\pi K}\,S_{K\pi}^{1,6} - S_{K\pi}^{3,6}\right) \\
&+ \frac{1}{96}(1+x_{\pi K})^2 S_{\eta K}^{1,2} + \frac{1}{16}(11+2x_{\pi K}-9x_{\eta K})S_{\eta K}^{1,3} \\
&- \frac{1}{16}(1+x_{\pi K})(5-2x_{\pi K}-3x_{\eta K})S_{\eta K}^{1,4} - \frac{1}{8}(1+x_{\pi K})S_{\eta K}^{2,1} \\
&+ \frac{1}{8}(1+x_{\pi K})S_{\eta K}^{2,2} + \frac{1}{4}(4-2x_{\pi K}+3x_{\eta K})S_{\eta K}^{2,3} \\
&- \frac{3}{8}(1-2x_{\pi K}+x_{\eta K})S_{\eta K}^{2,4} + \frac{3}{4}S_{\eta K}^{3,1} - \frac{3}{8}S_{\eta K}^{3,2} \\
&- \frac{3}{2}S_{\eta K}^{3,3} + 3\,S_{\eta K}^{3,5} \\
&+ \frac{3}{2}\left(x_{\pi K}\,S_{\eta K}^{1,5} - x_{\pi K}\,S_{\eta K}^{1,6} - S_{\eta K}^{3,6}\right)\Big\}.
\end{aligned}
\tag{D.25}
$$

The term appearing in Eq. (4.128) is

$$
\begin{aligned}
S^{(4)}(G_{K^\pm},\pi^\pm) = 2\,x_{\pi K}^{-1/2}\Big\{ & -\frac{3}{32}(1+x_{\pi K})^2 S_{K\pi}^{0,1} - \frac{3}{64}(1+x_{\pi K})^2 S_{K\pi}^{0,2} \\
& + \frac{3}{32}(1-2x_{\pi K})(3+x_{\pi K}) S_{K\pi}^{0,3} \\
& + \frac{3}{32}\left(1-x_{\pi K}^2\right) S_{K\pi}^{0,4} \\
& + \frac{3}{4}x_{\pi K}\, S_{K\pi}^{0,5} + \frac{3}{4}x_{\pi K}\, S_{K\pi}^{0,6} \\
& + \frac{5}{16}(1+x_{\pi K}) S_{K\pi}^{1,1} + \frac{5}{16}(1+x_{\pi K}) S_{K\pi}^{1,2} \\
& + \frac{1}{8}(3+8x_{\pi K}) S_{K\pi}^{1,3} - \frac{13}{16}(1-x_{\pi K}) S_{K\pi}^{1,4} \\
& + \frac{19}{16} S_{K\pi}^{2,2} + \frac{5}{4} S_{K\pi}^{2,3} + \frac{3}{4} S_{K\pi}^{2,6} \\
& - \frac{1}{96}(1+x_{\pi K})^2 S_{\eta K}^{0,1} - \frac{1}{192}(1+x_{\pi K})^2 S_{\eta K}^{0,2} \\
& - \frac{1}{32}(1-2x_{\pi K})(1-2x_{\pi K}-3x_{\eta K}) S_{\eta K}^{0,3} \\
& + \frac{1}{32}(1+x_{\pi K})(5-2x_{\pi K}-3x_{\eta K}) S_{\eta K}^{0,4} \\
& + \frac{3}{4}x_{\pi K}\, S_{\eta K}^{0,5} + \frac{3}{4}x_{\pi K}\, S_{\eta K}^{0,6} \\
& + \frac{1}{16}(1+x_{\pi K}) S_{\eta K}^{1,1} + \frac{1}{16}(1+x_{\pi K}) S_{\eta K}^{1,2} \\
& + \frac{1}{8}(1+4x_{\pi K}) S_{\eta K}^{1,3} - \frac{3}{16}(1-2x_{\pi K}+x_{\eta K}) S_{\eta K}^{1,4} \\
& + \frac{3}{16} S_{\eta K}^{2,2} + \frac{3}{4} S_{\eta K}^{2,3} + \frac{3}{4} S_{\eta K}^{2,6} \Big\}.
\end{aligned}
\tag{D.26}
$$

The term appearing in Eq. (4.129) is

$$
\begin{aligned}
S_D^{(4)}(G_{K^\pm},\pi^\pm) = 2\,x_{\pi K}^{-1/2}\Big\{ &+\frac{5}{16}(1+x_{\pi K})S_{K\pi}^{1,1}+\frac{1}{16}(1+x_{\pi K})(8+3x_{\pi K})S_{K\pi}^{1,2}\\
&+\frac{1}{8}(3+8x_{\pi K})S_{K\pi}^{1,3}\\
&-\frac{1}{8}(11-14x_{\pi K}-3x_{\pi K}^2)S_{K\pi}^{1,4}\\
&-\frac{3}{2}x_{\pi K}\,S_{K\pi}^{1,6}+\frac{3}{32}(1+x_{\pi K})^2S_{K\pi}^{1,7}\\
&-\frac{3}{16}(1-x_{\pi K}^2)S_{K\pi}^{1,8}-\frac{3}{2}x_{\pi K}\,S_{K\pi}^{1,9}\\
&+\frac{1}{8}(24+5x_{\pi K})S_{K\pi}^{2,2}+\frac{5}{2}S_{K\pi}^{2,3}\\
&+\frac{1}{4}(3+8x_{\pi K})S_{K\pi}^{2,4}+\frac{3}{2}S_{K\pi}^{2,6}\\
&+\frac{5}{8}(1+x_{\pi K})S_{K\pi}^{2,7}-\frac{13}{8}(1-x_{\pi K})S_{K\pi}^{2,8}\\
&-\frac{5}{2}S_{K\pi}^{3,4}-\frac{19}{8}S_{K\pi}^{3,7}-\frac{3}{2}S_{K\pi}^{3,9}\\
&+\frac{1}{16}(1+x_{\pi K})S_{\eta K}^{1,1}+\frac{1}{48}(1+x_{\pi K})(4+x_{\pi K})S_{\eta K}^{1,2}\\
&+\frac{1}{8}(1+4x_{\pi K})S_{\eta K}^{1,3}\\
&-\frac{1}{8}(1-x_{\pi K}+3x_{\eta K}-2x_{\pi K}^2-3x_{\pi K}x_{\eta K})S_{\eta K}^{1,4}\\
&-\frac{3}{2}x_{\pi K}\,S_{\eta K}^{1,6}+\frac{1}{96}(1+x_{\pi K})^2S_{\eta K}^{1,7}\\
&-\frac{1}{16}(1+x_{\pi K})(5-2x_{\pi K}-3x_{\eta K})S_{\eta K}^{1,8}-\frac{3}{2}x_{\pi K}\,S_{\eta K}^{1,9}\\
&+\frac{1}{8}(4+x_{\pi K})S_{\eta K}^{2,2}+\frac{3}{2}S_{\eta K}^{2,3}\\
&+\frac{1}{4}(1+4x_{\pi K})S_{\eta K}^{2,4}+\frac{3}{2}S_{\eta K}^{2,6}\\
&+\frac{1}{8}(1+x_{\pi K})S_{\eta K}^{2,7}-\frac{3}{8}(1-2x_{\pi K}+x_{\eta K})S_{\eta K}^{2,8}\\
&-\frac{3}{2}S_{\eta K}^{3,4}-\frac{3}{8}S_{\eta K}^{3,7}-\frac{3}{2}S_{\eta K}^{3,9}\Big\}.
\end{aligned}
\tag{D.27}
$$

The term appearing in Eq. (4.133) is

$$
\begin{aligned}
S^{(4)}(\vartheta_{\mathscr{G}_{K+}}) = x_{\pi K}^{-1}\Big\{ & + \frac{3}{16}(1+x_{\pi K})^2 S_{K\pi}^{1,1} + \frac{3}{32}(1+x_{\pi K})^2 S_{K\pi}^{1,2} \\
& - \frac{3}{16}(1-2x_{\pi K})(3+x_{\pi K}) S_{K\pi}^{1,3} \\
& - \frac{3}{16}(1-x_{\pi K}^2) S_{K\pi}^{1,4} \\
& - \frac{3}{2}x_{\pi K}\, S_{K\pi}^{1,5} - \frac{3}{2}x_{\pi K}\, S_{K\pi}^{1,6} \\
& + \frac{5}{8}(1+x_{\pi K}) S_{K\pi}^{2,1} + \frac{5}{8}(1+x_{\pi K}) S_{K\pi}^{2,2} \\
& + \frac{1}{4}(3+8x_{\pi K}) S_{K\pi}^{2,3} - \frac{13}{8}(1-x_{\pi K}) S_{K\pi}^{2,4} \\
& - \frac{3}{8} S_{K\pi}^{3,2} - \frac{5}{2} S_{K\pi}^{3,3} - \frac{3}{2} S_{K\pi}^{3,6} \\
& + \frac{1}{48}(1+x_{\pi K})^2 S_{\eta K}^{1,1} + \frac{1}{96}(1+x_{\pi K})^2 S_{\eta K}^{1,2} \\
& + \frac{1}{16}(1-2x_{\pi K})(1-2x_{\pi K}-3x_{\eta K}) S_{\eta K}^{1,3} \\
& - \frac{1}{16}(1+x_{\pi K})(5-2x_{\pi K}-3x_{\eta K}) S_{\eta K}^{1,4} \\
& - \frac{3}{2}x_{\pi K}\, S_{\eta K}^{1,5} - \frac{3}{2}x_{\pi K}\, S_{\eta K}^{1,6} \\
& + \frac{1}{8}(1+x_{\pi K}) S_{\eta K}^{2,1} + \frac{1}{8}(1+x_{\pi K}) S_{\eta K}^{2,2} \\
& + \frac{1}{4}(1+4x_{\pi K}) S_{\eta K}^{2,3} - \frac{3}{8}(1-2x_{\pi K}+x_{\eta K}) S_{\eta K}^{2,4} \\
& - \frac{3}{8} S_{\eta K}^{3,2} - \frac{3}{2} S_{\eta K}^{3,3} - \frac{3}{2} S_{\eta K}^{3,6} \Big\}.
\end{aligned}
\tag{D.28}
$$

D.3 Eta Meson

We present the term $S^{(4)}$ appearing in the asymptotic formula for the eta meson. Remark that the functions $T_{PQ}^{k,l}$ are defined in Eq. (D.30). In the next expressions, we denote the ratio of mass squares as $x_{PQ} = M_P^2/M_Q^2$ where $P, Q = \pi, K, \eta$.
The term appearing in Eq. (4.137) is

$$
S^{(4)}(M_\eta, \pi^\pm) = 2\left\{ \frac{x_{\pi\eta}^{3/2}}{3}\, T_{KK}^{0,1} - 2x_{\pi\eta}^{1/2}\, T_{KK}^{1,1} - 3x_{\pi\eta}^{-1/2}\, T_{KK}^{2,1} + \frac{2}{9}x_{\pi\eta}^{3/2}\, T_{\eta\pi}^{0,1} \right\}. \tag{D.29}
$$

The functions $S_{PQ}^{k,l}$, $T_{PQ}^{k,l}$ entering the expressions for kaons and eta meson are defined as

$$\begin{aligned} S^{k,l}_{PQ} &= S^{k,l}_{PQ}(\lambda_\pi|\vec{n}|) \\ &= \begin{cases} \mathrm{Re} \\ \mathrm{Im} \end{cases} N x_{\pi K}^{(k+1)/2} \int_{\mathbb{R}} \mathrm{d}y\, y^k \mathrm{e}^{-\lambda_\pi|\vec{n}|\sqrt{1+y^2}} g^{(l)}_{PQ}(M_K^2 + M_\pi^2 + 2iM_K M_\pi y) \\ &\qquad \text{for} \begin{cases} k \text{ even} \\ k \text{ odd} \end{cases} \\ T^{k,l}_{PQ} &= T^{k,l}_{PQ}(\lambda_\pi|\vec{n}|) \\ &= \begin{cases} \mathrm{Re} \\ \mathrm{Im} \end{cases} N x_{\pi \eta}^{(k+1)/2} \int_{\mathbb{R}} \mathrm{d}y\, y^k \mathrm{e}^{-\lambda_\pi|\vec{n}|\sqrt{1+y^2}} g^{(l)}_{PQ}(M_\eta^2 + M_\pi^2 + 2iM_\eta M_\pi y) \\ &\qquad \text{for} \begin{cases} k \text{ even} \\ k \text{ odd.} \end{cases} \end{aligned} \tag{D.30}$$

Here, $N = (4\pi)^2$ and

$$\begin{array}{lll} g^{(1)}_{PQ}(x) = \bar{J}_{PQ}(x) & g^{(2)}_{PQ}(x) = M_K^2\, \bar{J}'_{PQ}(x) & g^{(7)}_{PQ}(x) = M_K^4\, \bar{J}''_{PQ}(x) \\ g^{(3)}_{PQ}(x) = K_{PQ}(x) & g^{(4)}_{PQ}(x) = M_K^2\, K'_{PQ}(x) & g^{(8)}_{PQ}(x) = M_K^4\, K''_{PQ}(x) \\ g^{(5)}_{PQ}(x) = \bar{M}_{PQ}(x) & g^{(6)}_{PQ}(x) = M_K^2\, \bar{M}'_{PQ}(x) & g^{(9)}_{PQ}(x) = M_K^4\, \bar{M}''_{PQ}(x). \end{array} \tag{D.31}$$

The explicit forms of $g^{(l)}_{PQ}(x)$ were presented in Ref. [48]. They can be expressed in terms of the loop-integral function $\bar{J}_{PQ}(q^2) = J_{PQ}(q^2) - J_{PQ}(0)$ evaluated in $d = 4$ dimensions,

$$J_{PQ}(q^2) = \int \frac{\mathrm{d}^d k}{(2\pi)^d} \frac{1}{i\big[M_P^2 - (k+q)^2\big]\big[M_Q^2 - k^2\big]}. \tag{D.32}$$

Using the abbreviations,

$$\begin{array}{lll} \bar{J}(t) = \bar{J}_{PQ}(t) & t = q^2 & \Delta = M^2 - m^2 \\ K(t) = K_{PQ}(t) & M = M_P & \Sigma = M^2 + m^2 \\ \bar{M}(t) = \bar{M}_{PQ}(t) & m = M_Q & \rho = (t+\Delta)^2 - 4tM^2, \end{array} \tag{D.33}$$

the above functions take the forms

$$\begin{aligned} \bar{J}(t) &= \frac{1}{2N}\left[2 + \frac{\Delta}{t}\ln\frac{m^2}{M^2} - \frac{\Sigma}{\Delta}\ln\frac{m^2}{M^2} - \frac{\sqrt{\rho}}{t}\ln\frac{(t+\sqrt{\rho})^2 - \Delta^2}{(t-\sqrt{\rho})^2 - \Delta^2}\right] \\ K(t) &= \frac{\Delta}{2t}\bar{J}(t) \\ \bar{M}(t) &= \frac{1}{12t}[t - 2\Sigma]\bar{J}(t) + \frac{\Delta^2}{3t^2}\bar{J}(t) + \frac{1}{18N} - \frac{1}{6Nt}\left[\Sigma + \frac{2M^2m^2}{\Delta}\ln\frac{m^2}{M^2}\right]. \end{aligned} \tag{D.34}$$

We conclude with a remark on the analycity of the loop-integral functions. In the asymptotic formulae the loop-integral functions are evaluated in the complex plane along the imaginary axis. Eq. (D.34) represents an analytic continuation for the loop-integral functions to the complex plane. In one case the representation (D.34) is not an unambigous analytic continuation: for $\bar{J}_{PQ}(M_P^2 + M_Q^2 + 2iM_P M_Q y)$ due to the negative value of $\rho = -4M_P^2 M_Q^2(1+y^2)$. In Ref. [32] an analytic continuation was proposed but it was not fully correct. Here, we give the correct analytic continuation. One must take the positive value of the square root,

$$\sqrt{\rho} = 2iM_P M_Q \sqrt{1+y^2}, \tag{D.35}$$

for which the logarithm in (D.34) becomes

$$\ln \frac{(t+\sqrt{\rho})^2 - \Delta^2}{(t-\sqrt{\rho})^2 - \Delta^2} = \ln \frac{(1+y^2)^{\frac{1}{2}} + y}{(1+y^2)^{\frac{1}{2}} - y} + i\pi, \qquad \text{for all } y \in \mathbb{R}, \tag{D.36}$$

with $t = M_P^2 + M_Q^2 + 2iM_P M_Q\, y$.

Bibliography

[1] K. G. Wilson, "Confinement of Quarks," *Phys. Rev.*, vol. D10, pp. 2445–2459, 1974.

[2] K. Olive *et al.*, "Review of Particle Physics," *Chin. Phys.*, vol. C38, p. 090001, 2014.

[3] E. Fermi, "Tentativo di una Teoria dell'Emissione dei Raggi 'Beta'," *La Ricerca scientifica*, vol. 2, no. 12, 1933.

[4] E. Fermi, "Tentativo di una Teoria dei Raggi β," *Nuovo Cim.*, vol. 11, no. 1, pp. 1–19, 1934.

[5] E. Fermi, "Versuch einer Theorie der β-Strahlen. 1.," *Zeitschrift für Physik*, vol. 88, no. 3-4, pp. 161–177, 1934.

[6] H. Euler, "Über die Streuung von Licht an Licht nach der Diracschen Theorie," *Annalen der Physik*, vol. 418, no. 5, pp. 398–448, 1936.

[7] H. Euler and W. Heisenberg, "Folgerungen aus der Diracschen Theorie des Positrons," *Zeitschrift für Physik*, vol. 98, no. 11-12, pp. 714–732, 1936.

[8] T. Appelquist and J. Carazzone, "Infrared Singularities and Massive Fields," *Phys. Rev.*, vol. D11, p. 2856, 1975.

[9] S. Weinberg, "Phenomenological Lagrangians," *Physica*, vol. A96, p. 327, 1979.

[10] J. Gasser and H. Leutwyler, "Chiral Perturbation Theory to One Loop," *Ann. Phys.*, vol. 158, p. 142, 1984.

[11] J. Gasser and H. Leutwyler, "Chiral Perturbation Theory: Expansions in the Mass of the Strange Quark," *Nucl. Phys.*, vol. B250, p. 465, 1985.

[12] J. Gasser, M. E. Sainio, and A. Svarc, "Nucleons with Chiral Loops," *Nucl. Phys.*, vol. B307, p. 779, 1988.

[13] E. E. Jenkins and A. V. Manohar, "Baryon Chiral Perturbation Theory Using a Heavy Fermion Lagrangian," *Phys. Lett.*, vol. B255, pp. 558–562, 1991.

[14] V. Bernard, N. Kaiser, and U.-G. Meissner, "Chiral Dynamics in Nucleons and Nuclei," *Int. J. Mod. Phys.*, vol. E4, pp. 193–346, 1995.

[15] T. Becher and H. Leutwyler, “Baryon Chiral Perturbation Theory in Manifestly Lorentz Invariant Form,” *Eur. Phys. J.*, vol. C9, pp. 643–671, 1999.

[16] S. Weinberg, “Nuclear Forces from Chiral Lagrangians,” *Phys. Lett.*, vol. B251, pp. 288–292, 1990.

[17] S. Weinberg, “Effective Chiral Lagrangians for Nucleon - Pion Interactions and Nuclear Forces,” *Nucl. Phys.*, vol. B363, pp. 3–18, 1991.

[18] S. Weinberg, “Three-Body Interactions among Nucleons and Pions,” *Phys. Lett.*, vol. B295, pp. 114–121, 1992.

[19] J. Gasser and H. Leutwyler, “Light Quarks at Low Temperatures,” *Phys. Lett.*, vol. B184, p. 83, 1987.

[20] J. Gasser and H. Leutwyler, “Thermodynamics of Chiral Symmetry,” *Phys. Lett.*, vol. B188, p. 477, 1987.

[21] J. Gasser and H. Leutwyler, “Spontaneously Broken Symmetries: Effective Lagrangians at Finite Volume,” *Nucl. Phys.*, vol. B307, p. 763, 1988.

[22] M. Lüscher, “On a Relation between Finite Size Effects and Elastic Scattering Processes,” 1983. Lecture given at Cargèse Summer Inst., Cargèse, France, Sep. 1-15.

[23] M. Lüscher, “Volume Dependence of the Energy Spectrum in Massive Quantum Field Theories. 1. Stable Particle States,” *Commun. Math. Phys.*, vol. 104, p. 177, 1986.

[24] G. Colangelo, S. Dürr, and R. Sommer, “Finite Size Effects on M_π in QCD from Chiral Perturbation Theory,” *Nucl. Phys. Proc. Suppl.*, vol. 119, pp. 254–256, 2003.

[25] G. Colangelo and S. Dürr, “The Pion Mass in Finite Volume,” *Eur. Phys. J.*, vol. C33, pp. 543–553, 2004.

[26] G. Colangelo, U. Wenger, and J. M. Wu, “Twisted Mass Finite Volume Effects,” *Phys. Rev.*, vol. D82, p. 034502, 2010.

[27] A. Ali Khan *et al.*, “The Nucleon Mass in $N_\mathrm{f} = 2$ Lattice QCD: Finite Size Effects from Chiral Perturbation Theory,” *Nucl. Phys.*, vol. B689, pp. 175–194, 2004.

[28] Y. Koma and M. Koma, “On the Finite Size Mass Shift Formula for Stable Particles,” *Nucl. Phys.*, vol. B713, pp. 575–597, 2005.

[29] G. Colangelo, A. Fuhrer, and C. Häfeli, “The Pion and Proton Mass in Finite Volume,” *Nucl. Phys. Proc. Suppl.*, vol. 153, pp. 41–48, 2006.

[30] G. Colangelo, A. Fuhrer, and S. Lanz, “Finite Volume Effects for Nucleon and Heavy Meson Masses,” *Phys. Rev.*, vol. D82, p. 034506, 2010.

[31] G. Colangelo and C. Häfeli, "An Asymptotic Formula for the Pion Decay Constant in a Large Volume," *Phys. Lett.*, vol. B590, pp. 258–264, 2004.

[32] G. Colangelo, S. Dürr, and C. Häfeli, "Finite Volume Effects for Meson Masses and Decay Constants," *Nucl. Phys.*, vol. B721, pp. 136–174, 2005.

[33] G. de Divitiis, R. Petronzio, and N. Tantalo, "On the Discretization of Physical Momenta in Lattice QCD," *Phys. Lett.*, vol. B595, pp. 408–413, 2004.

[34] G. M. de Divitiis and N. Tantalo, "Non-leptonic Two-Body Decay Amplitudes from Finite Volume Calculations," 2004.

[35] D. Guadagnoli, F. Mescia, and S. Simula, "Lattice Study of Semileptonic Form Factors with Twisted Boundary Conditions," *Phys. Rev.*, vol. D73, p. 114504, 2006.

[36] C. T. Sachrajda and G. Villadoro, "Twisted Boundary Conditions in Lattice Simulations," *Phys. Lett.*, vol. B609, pp. 73–85, 2005.

[37] F.-J. Jiang and B. C. Tiburzi, "Flavor Twisted Boundary Conditions, Pion Momentum, and the Pion Electromagnetic Form Factor," *Phys. Lett.*, vol. B645, pp. 314–321, 2007.

[38] J. Bijnens and J. Relefors, "Masses, Decay Constants and Electromagnetic Form Factors with Twisted Boundary Conditions," 2014.

[39] H. Hellmann, *Einführung in die Quantenchemie*, p. 285. Leipzig: Franz Deuticke, 1937.

[40] R. P. Feynman, "Forces in Molecules," *Phys. Rev.*, vol. 56, pp. 340–343, 1939.

[41] H. Green, "A Prerenormalized Quantum Electrodynamics," *Proc. Phys. Soc.*, vol. A66, pp. 873–880, 1953.

[42] Y. Takahashi *Nuovo Cim.*, vol. Ser 10, p. 370, 1957.

[43] Y. Takahashi, "On the Generalized Ward Identity," *Nuovo Cim.*, vol. 6, p. 371, 1957.

[44] J. Bijnens, G. Colangelo, G. Ecker, J. Gasser, and M. Sainio, "Pion-Pion Scattering at Low Energy," *Nucl. Phys.*, vol. B508, pp. 263–310, 1997.

[45] V. Bernard, N. Kaiser, and U. G. Meissner, "πK-Scattering in Chiral Perturbation Theory to One Loop," *Nucl. Phys.*, vol. B357, pp. 129–152, 1991.

[46] V. Bernard, N. Kaiser, and U. G. Meissner, "$\pi\eta$-Scattering in QCD," *Phys. Rev.*, vol. D44, pp. 3698–3701, 1991.

[47] G. Colangelo, M. Finkemeier, and R. Urech, "Tau Decays and Chiral Perturbation Theory," *Phys. Rev.*, vol. D54, pp. 4403–4418, 1996.

[48] J. Bijnens, G. Colangelo, and J. Gasser, "$K_{\ell 4}$-Decays Beyond One Loop," *Nucl. Phys.*, vol. B427, pp. 427–454, 1994.

[49] S. Aoki *et al.*, "2+1 Flavor Lattice QCD toward the Physical Point," *Phys. Rev.*, vol. D79, p. 034503, 2009.

[50] S. Aoki *et al.*, "Physical Point Simulation in 2+1 Flavor Lattice QCD," *Phys. Rev.*, vol. D81, p. 074503, 2010.

[51] R. Baron *et al.*, "Light Hadrons from Lattice QCD with Light (u, d), Strange and Charm Dynamical Quarks," *JHEP*, vol. 06, p. 111, 2010.

[52] J. Hu, F.-J. Jiang, and B. C. Tiburzi, "Current Renormalization in Finite Volume," *Phys. Lett.*, vol. B653, pp. 350–357, 2007.

[53] H. Georgi, "Effective Field Theory," *Ann. Rev. Nucl. Part. Sci.*, vol. 43, pp. 209–252, 1993.

[54] A. Pich, "Effective Field Theory: Course," pp. 949–1049, 1998.

[55] G. Ecker, "Effective Field Theories," 2005.

[56] C. Burgess, "Introduction to Effective Field Theory," *Ann. Rev. Nucl .Part. Sci.*, vol. 57, pp. 329–362, 2007.

[57] S. Weinberg, "Effective Field Theory, Past and Future," *PoS*, vol. CD09, p. 001, 2009.

[58] H. Leutwyler, "On the Foundations of Chiral Perturbation Theory," *Ann. Phys.*, vol. 235, pp. 165–203, 1994.

[59] E. D'Hoker and S. Weinberg, "General Effective Actions," *Phys. Rev.*, vol. D50, pp. 6050–6053, 1994.

[60] H. Fritzsch, M. Gell-Mann, and H. Leutwyler, "Advantages of the Color Octet Gluon Picture," *Phys. Lett.*, vol. B47, pp. 365–368, 1973.

[61] S. Weinberg, "Non-abelian Gauge Theories of the Strong Interactions," *Phys. Rev. Lett.*, vol. 31, pp. 494–497, 1973.

[62] S. Scherer, "Introduction to Chiral Perturbation Theory," *Adv. Nucl. Phys.*, vol. 27, p. 277, 2003.

[63] "First Combination of Tevatron and LHC Measurements of the t-Quark Mass," 2014.

[64] D. Gross and F. Wilczek, "Ultraviolet Behavior of Non-abelian Gauge Theories," *Phys. Rev. Lett.*, vol. 30, pp. 1343–1346, 1973.

[65] D. Gross and F. Wilczek, "Asymptotically Free Gauge Theories. 1.," *Phys. Rev.*, vol. D8, pp. 3633–3652, 1973.

[66] H. Politzer, "Reliable Perturbative Results for Strong Interactions?," *Phys. Rev. Lett.*, vol. 30, pp. 1346–1349, 1973.

[67] D. Gross and F. Wilczek, "Asymptotically Free Gauge Theories. 2.," *Phys. Rev.*, vol. D9, pp. 980–993, 1974.

[68] D. J. Gross, "Twenty Five Years of Asymptotic Freedom," *Nucl. Phys. Proc. Suppl.*, vol. 74, pp. 426–446, 1999.

[69] F. Wilczek, "Asymptotic Freedom: from Paradox to Paradigm," *Proc. Nat. Acad. Sci.*, vol. 102, pp. 8403–8413, 2005. Lecture given in acceptance of the Nobel Prize, Dec. 2004.

[70] A. M. Jaffe and E. Witten, "Quantum Yang–Mills Theory," 2000. Clay Mathematics Institute Millenium Prize problem.

[71] E. Noether, "Invariant Variation Problems," *Gott. Nachr.*, vol. 1918, pp. 235–257, 1918.

[72] S. L. Adler, "Axialvector Vertex in Spinor Electrodynamics," *Phys. Rev.*, vol. 177, pp. 2426–2438, 1969.

[73] S. L. Adler and W. A. Bardeen, "Absence of Higher Order Corrections in the Anomalous Axialvector Divergence Equation," *Phys. Rev.*, vol. 182, pp. 1517–1536, 1969.

[74] W. A. Bardeen, "Anomalous Ward Identities in Spinor Field Theories," *Phys. Rev.*, vol. 184, pp. 1848–1857, 1969.

[75] J. Bell and R. Jackiw, "A PCAC Puzzle: $\pi^0 \to \gamma\gamma$ in the Sigma Model," *Nuovo Cim.*, vol. A60, pp. 47–61, 1969.

[76] M. Gell-Mann and Y. Neemam, "The Eightfold Way: a Review with a Collection of Reprints," 1964. W. A. Benjamin, Publisher (QCD161:G4).

[77] Y. Nambu, "Axialvector Current Conservation in Weak Interactions," *Phys. Rev. Lett.*, vol. 4, pp. 380–382, 1960.

[78] Y. Nambu and G. Jona-Lasinio, "Dynamical Model of Elementary Particles Based on an Analogy with Superconductivity. 1.," *Phys. Rev.*, vol. 122, pp. 345–358, 1961.

[79] Y. Nambu and G. Jona-Lasinio, "Dynamical Model of Elementary Particles Based on an Analogy with Superconductivity. 2.," *Phys. Rev.*, vol. 124, pp. 246–254, 1961.

[80] P. Stoffer, "A Dispersive Treatment of $K_{\ell 4}$ Decays," master thesis, 2010.

[81] J. Goldstone, "Field Theories with Superconductor Solutions," *Nuovo Cim.*, vol. 19, pp. 154–164, 1961.

[82] J. Goldstone, A. Salam, and S. Weinberg, "Broken Symmetries," *Phys. Rev.*, vol. 127, pp. 965–970, 1962.

[83] S. R. Coleman and E. Witten, "Chiral Symmetry Breakdown in Large N_c Chromodynamics," *Phys. Rev. Lett.*, vol. 45, p. 100, 1980.

[84] G. 't Hooft, C. Itzykson, A. Jaffe, H. Lehmann, P. Mitter, *et al.*, "Recent Developments in Gauge Theories. Proceedings, Nato Advanced Study Institute, Cargèse, France, August 26 - September 8, 1979," *NATO Sci. Ser. B*, vol. 59, pp. pp.1–438, 1980.

[85] C. Vafa and E. Witten, "Restrictions on Symmetry Breaking in Vector-Like Gauge Theories," *Nucl. Phys.*, vol. B234, p. 173, 1984.

[86] S. Aoki, Y. Aoki, C. Bernard, T. Blum, G. Colangelo, *et al.*, "Review of Lattice Results Concerning Low-Energy Particle Physics," *Eur. Phys. J.*, vol. C74, no. 9, p. 2890, 2014.

[87] A. Bazavov, C. Bernard, C. DeTar, X. Du, W. Freeman, *et al.*, "Staggered Chiral Perturbation Theory in the Two-Flavor case and SU(2) Analysis of the MILC Data," *PoS*, vol. LATTICE2010, p. 083, 2010.

[88] Y. Aoki *et al.*, "Continuum Limit Physics from $(2+1)$-Flavor Domain Wall QCD," *Phys. Rev.*, vol. D83, p. 074508, 2011.

[89] S. Borsanyi, S. Durr, Z. Fodor, S. Krieg, A. Schafer, *et al.*, "SU(2) Chiral Perturbation Theory Low-Energy Constants from $(2+1)$-Flavor Staggered Lattice Simulations," *Phys. Rev.*, vol. D88, p. 014513, 2013.

[90] H. Leutwyler, "Introduction to Chiral Perturbation Theory," 2008. Lectures given at Summer School on Flavor Physics, Benasque, July 13-17.

[91] B. Borasoy, "Introduction to Chiral Perturbation Theory," pp. 1–26, 2007.

[92] B. Kubis, "An Introduction to Chiral Perturbation Theory," 2007.

[93] J. Wess and B. Zumino, "Consequences of Anomalous Ward Identities," *Phys. Lett.*, vol. B37, p. 95, 1971.

[94] E. Witten, "Global Aspects of Current Algebra," *Nucl. Phys.*, vol. B223, pp. 422–432, 1983.

[95] S. Weinberg, "Non-linear Realizations of Chiral Symmetry," *Phys. Rev.*, vol. 166, pp. 1568–1577, 1968.

[96] S. R. Coleman, J. Wess, and B. Zumino, “Structure of Phenomenological Lagrangians. 1.,” *Phys. Rev.*, vol. 177, pp. 2239–2247, 1969.

[97] C. G. Callan, Jr., S. R. Coleman, J. Wess, and B. Zumino, “Structure of Phenomenological Lagrangians. 2.,” *Phys. Rev.*, vol. 177, pp. 2247–2250, 1969.

[98] M. Gell-Mann and M. Levy, “The Axial Vector Current in Beta Decay,” *Nuovo Cim.*, vol. 16, p. 705, 1960.

[99] J. Bernstein, S. Fubini, M. Gell-Mann, and W. Thirring, “On the Decay Rate of the Charged Pion,” *Nuovo Cim.*, vol. 17, no. 5, pp. 757–766, 1960.

[100] K.-C. Chou, “On the Pseudovector Current and Lepton Decays of Baryons and Mesons,” *Soviet Physics JETP*, vol. 12, p. 492, 1961.

[101] R. Akhoury and A. Alfakih, “Invariant Background Field Method for Chiral Lagrangians Including Wess–Zumino Terms,” *Ann. Phys.*, vol. 210, pp. 81–111, 1991.

[102] J. Bijnens, G. Colangelo, and G. Ecker, “The Mesonic Chiral Lagrangian of Order p^6,” *JHEP*, vol. 9902, p. 020, 1999.

[103] J. Bijnens, L. Girlanda, and P. Talavera, “The Anomalous Chiral Lagrangian of Order p^6,” *Eur. Phys. J.*, vol. C23, pp. 539–544, 2002. 12 pages, misprint in table 2 corrected Report-no: LU TP 01-34, DFPD-01/TH/25, CPT-2001/P.4256 Journal-ref: Eur.Phys.J. C23 (2002) 539-544.

[104] T. Ebertshauser, H. Fearing, and S. Scherer, “The Anomalous Chiral Perturbation Theory Meson Lagrangian to Order p^6 Revisited,” *Phys. Rev.*, vol. D65, p. 054033, 2002.

[105] H. Fearing and S. Scherer, “Extension of the Chiral Perturbation Theory Meson Lagrangian to Order p^6,” *Phys. Rev.*, vol. D53, pp. 315–348, 1996.

[106] C. Häfeli, M. A. Ivanov, M. Schmid, and G. Ecker, “On the Mesonic Lagrangian of order p^6 in Chiral SU(2),” 2007.

[107] J. Bijnens, “Status of Strong ChPT,” *PoS*, vol. EFT09, p. 022, 2009.

[108] S. Weinberg, “High-Energy Behavior in Quantum Field Theory,” *Phys. Rev.*, vol. 118, pp. 838–849, 1960.

[109] G. Ecker, “Chiral Perturbation Theory,” *Prog. Part. Nucl. Phys.*, vol. 35, pp. 1–80, 1995.

[110] M. Gell-Mann, R. Oakes, and B. Renner, “Behavior of Current Divergences under $SU(3) \times SU(3)$,” *Phys. Rev.*, vol. 175, pp. 2195–2199, 1968.

[111] S. Okubo, "Note on Unitary Symmetry in Strong Interactions," *Prog. Theor. Phys.*, vol. 27, pp. 949–966, 1962.

[112] S. Okubo, "Note on Unitary Symmetry in Strong Interaction. 2. Excited States of Baryons," *Prog. Theor. Phys.*, vol. 28, pp. 24–32, 1962.

[113] A. Manohar and H. Georgi, "Chiral Quarks and the Non-relativistic Quark Model," *Nucl. Phys.*, vol. B234, p. 189, 1984.

[114] J. C. Ward, "An Identity in Quantum Electrodynamics," *Phys. Rev.*, vol. 78, p. 182, 1950.

[115] J. Bijnens, G. Colangelo, and P. Talavera, "The Vector and Scalar Form Factors of the Pion to Two Loops," *JHEP*, vol. 05, p. 014, 1998.

[116] G. Colangelo, "Finite Volume Effects in Chiral Perturbation Theory," *Nucl. Phys. Proc. Suppl.*, vol. 140, pp. 120–126, 2005.

[117] P. Hasenfratz and H. Leutwyler, "Goldstone Boson Related Finite Size Effects in Field Theory and Critical Phenomena with $\mathrm{O}(N)$ Symmetry," *Nucl. Phys.*, vol. B343, pp. 241–284, 1990.

[118] F. Hansen, "Finite Size Effects in Spontaneously Broken $\mathrm{SU}(N) \times \mathrm{SU}(N)$ Theories," *Nucl. Phys.*, vol. B345, pp. 685–708, 1990.

[119] F. Hansen and H. Leutwyler, "Charge Correlations and Topological Susceptibility in QCD," *Nucl. Phys.*, vol. B350, pp. 201–227, 1991.

[120] C. Häfeli, 2008. Private communications and notes.

[121] S. Aoki *et al.*, "Pion Form Factors from Two-Flavor Lattice QCD with Exact Chiral Symmetry," *Phys. Rev.*, vol. D80, p. 034508, 2009.

[122] T. B. Bunton, F.-J. Jiang, and B. C. Tiburzi, "Extrapolations of Lattice Meson Form Factors," *Phys. Rev.*, vol. D74, p. 034514, 2006.

[123] B. Borasoy and R. Lewis, "Volume Dependences from Lattice Chiral Perturbation Theory," *Phys. Rev.*, vol. D71, p. 014033, 2005.

[124] K. Ghorbani, "Chiral and Volume Extrapolation of Pion and Kaon Electromagnetic Form Factor within SU(3) ChPT," 2011.

[125] R. A. Briceno, Z. Davoudi, T. C. Luu, and M. J. Savage, "Two-Baryon Systems with Twisted Boundary Conditions," *Phys. Rev.*, vol. D89, no. 7, p. 074509, 2014.

[126] B. C. Tiburzi, "External Momentum, Volume Effects, and the Nucleon Magnetic Moment," *Phys. Rev.*, vol. D77, p. 014510, 2008.

[127] J. Hall, D. Leinweber, B. Owen, and R. Young, "Finite Volume Corrections to Charge Radii," *Phys. Lett.*, vol. B725, pp. 101–105, 2013.

[128] B. C. Tiburzi, "Finite Volume Effects on the Extraction of Form Factors at Zero Momentum," *Phys. Rev.*, vol. D90, no. 5, p. 054508, 2014.

[129] B. C. Tiburzi, "Volume Effects on the Method of Extracting Form Factors at Zero Momentum," *PoS*, vol. LATTICE2014, p. 132, 2015.

[130] Y. Koma and M. Koma, "Finite Size Mass Shift Formula for Stable Particles Revisited," *Nucl. Phys. Proc. Suppl.*, vol. 140, pp. 329–331, 2005. [, 329 (2004)].

[131] Y. Koma and M. Koma, "More on the Finite Size Mass Shift Formula for Stable Particles," 2005.

[132] H. Leutwyler, "QCD: Low Temperature Expansion and Finite Size Effects," *Nucl. Phys. Proc. Suppl.*, vol. 4, p. 248, 1988.

[133] C. Häfeli, "Finite Volume Effects in Chiral Perturbation Theory," phd thesis, 2005.

[134] J. Bijnens, P. Dhonte, and P. Talavera, "πK-Scattering in Three-Flavor ChPT," *JHEP*, vol. 0405, p. 036, 2004.

[135] J. Bijnens and I. Jemos, "A New Global Fit of the L_i^r at Next-to-Next-to-Leading Order in Chiral Perturbation Theory," *Nucl. Phys.*, vol. B854, pp. 631–665, 2012.

[136] G. Colangelo, J. Gasser, and H. Leutwyler, "$\pi\pi$-Scattering," *Nucl. Phys.*, vol. B603, pp. 125–179, 2001.

[137] A. Bazavov *et al.*, "MILC Results for Light Pseudoscalars," *PoS*, vol. CD09, p. 007, 2009.

[138] R. Arthur *et al.*, "Domain Wall QCD with Near-Physical Pions," *Phys. Rev.*, vol. D87, p. 094514, 2013.

[139] S. Beane, W. Detmold, P. Junnarkar, T. Luu, K. Orginos, *et al.*, "SU(2) Low-Energy Constants from Mixed-Action Lattice QCD," *Phys. Rev.*, vol. D86, p. 094509, 2012.

[140] A. Bazavov *et al.*, "Results for Light Pseudoscalar Mesons," *PoS*, vol. LATTICE2010, p. 074, 2010.

[141] E. Follana, C. Davies, G. Lepage, and J. Shigemitsu, "High Precision Determination of the π, K, D and D_s Decay Constants from Lattice QCD," *Phys. Rev. Lett.*, vol. 100, p. 062002, 2008.

[142] N. Nakanishi, *Graph Theory and Feynman Integrals.* New York: Gordon and Breach, 1971.

Erklärung

gemäss Art. 28 Abs. 2 RSL 05

Name, Vorname:	Vaghi, Alessio
Matrikelnummer:	99-915-738
Studiengang:	Physik
	Bachelor ☐ Master ☐ Dissertation ☒
Titel der Arbeit:	Finite Volume Effects in Chiral Perturbation Theory with Twisted Boundary Conditions
Leiter der Arbeit:	Prof. Dr. Colangelo Gilberto

Ich erkläre hiermit, dass ich diese Arbeit selbständig verfasst und keine anderen als die angegebenen Quellen benutzt habe. Alle Stellen, die wörtlich oder sinngemäss aus Quellen entnommen wurden, habe ich als solche gekennzeichnet. Mir ist bekannt, dass andernfalls der Senat gemäss Artikel 36 Absatz 1 Buchstabe r des Gesetzes vom 5. September 1996 über die Universität zum Entzug des auf Grund dieser Arbeit verliehenen Titels berechtigt ist. Ich gewähre hiermit Einsicht in diese Arbeit.

Bern, den 2. November 2015

Alessio Vaghi

Curriculum Vitae

Personal Information

Name	**Alessio Giovanni Willy Vaghi**
Date of birth	February 14, 1980
Nationality	Swiss
Civil status	Celibate
Present address	Institute for Theoretical Physics University of Bern Sidlerstrasse 5 3012 Bern, Switzerland Phone: +41 31 631 86 29 Email: `vaghial@itp.unibe.ch`

Education

2007—2015	University of Bern Ph.D. student of Prof. Dr. G. Colangelo
1999—2006	ETH (Swiss Federal Institute of Technology) Zurich Studies in Physics and Mathematics Degree in Theoretical Physics (Master of Science in Physics): *Localization and Spectral Fluctuations* supervised by Prof. Dr. G. M. Graf
1995—1999	“Liceo Cantonale” of Mendrisio Scientific Maturity Diplom
1986—1995	Schools in Chiasso

Working Experiences

2015	Teaching assistant in Department of Theoretical Physics at University of Bern
2014—2015	Teaching assistant in Department of Physics and Astronomy at University of Bern Substitute teacher of Physics and Mathematics at “Liceo Cantonale” of Mendrisio and at “Centro Professionale Commerciale” of Lugano
2007—2012	Teaching assistant in Department of Theoretical Physics at University of Bern
2007	Teaching assistant in Department of Mathematics at ETH Zurich

Workshops and PhD-Schools

June 2010	FLAVIAnet summer school on Flavor Physics in Bern, Switzerland
July 2009	*Chiral Dynamics*, International workshop in Bern, Switzerland
February 2009	*Effective Field Theories: from the Pion to the Upsilon*, International workshop in Valencia, Spain
July 2008	FLAVIAnet summer school on Flavor Physics in Benasque, Spain
January 2008	CHIPP winter school on Particles Physics in Näfels, Switzerland

Publication

A Remark on the Estimate of a Determinant by Minami,
G. M. Graf, A. Vaghi, Lett. Math. Phys. 79 (2007) 17-22,
arXiv: `math-ph/0604033`

Languages

Italian	Mother tongue
English	Good skills in spoken and written
German	Good skills in spoken and written
French	Good skills in spoken and written